

John please

U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

SEARCH REQUEST FORM

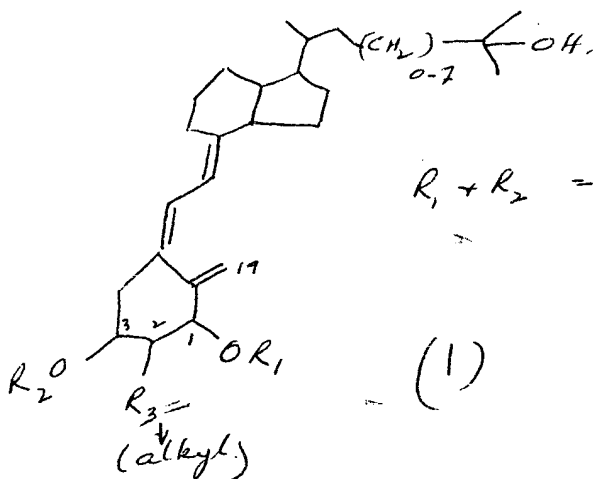
6-717

Requestor's Name: Qazi, SabihaSerial Number: 09/214,155Date: 6/22/99Phone: 305-3910Art Unit: 16163307

Search Topic:

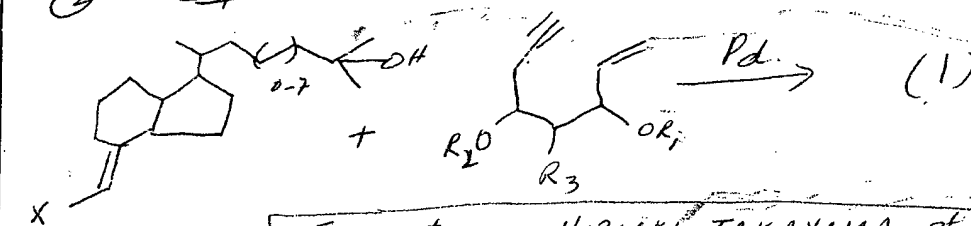
Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).

Please search for

① 1,25-dehydroxy-2-methylvitamin D₃ of for (1)

Point of Contact:
John Dantzman
Technical Info. Specialist
CM1 1E05 Tel: 308-4488

② Preparation:

Inventors: HIROAKI TAKAYAMA et al.Priority: JP 9-114695 5/2/97

STAFF USE ONLY

Date completed: 6-22-99
 Searcher: JUN D.
 Terminal time: 00 40
 Elapsed time: _____
 CPU time: _____
 Total time: 60
 Number of Searches: _____
 Number of Databases: _____

Search Site

☐ STIC
☒ CM-1
☐ Pre-S

Type of Search

☐ N.A. Sequence
☒ A.A. Sequence
☐ Structure
☐ Bibliographic

Vendors

☒ IG
☐ STN
☐ Dialog
☐ APS
☐ Geninfo
☐ SDC
☐ DARC/Questel
☐ Other

SUMMARY

QAZI

09/214155

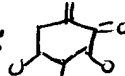
Page 1

=> d his

(FILE 'REGISTRY' ENTERED AT 14:07:07 ON 22 JUN 1999)

L1 DEL HIS Y
L2 STR
L3 1 S L1
L4 STR L1
L5 1 S L3
L6 36 S L3 FUL
L7 STR L3
L8 2 S L5 NOT 46.150.1/RID
34 S L5 NOT L7

product + Reactant

this eliminates: 

Reactant

product

FILE 'CAPLUS' ENTERED AT 14:57:26 ON 22 JUN 1999

FILE 'REGISTRY' ENTERED AT 14:57:49 ON 22 JUN 1999

FILE 'CAPLUS' ENTERED AT 14:58:44 ON 22 JUN 1999

FILE 'HCAPLUS' ENTERED AT 15:00:14 ON 22 JUN 1999

L9 11 S L8
L10 9 S L7
L11 4 S L9 AND L10
SELECT RN L11 1-4

4 references

FILE 'REGISTRY' ENTERED AT 15:00:41 ON 22 JUN 1999

L12 109 S E97-205
L13 89 S L12 NOT L5

FILE 'HCAPLUS' ENTERED AT 15:03:36 ON 22 JUN 1999

L14 4 S L9 AND L10 AND L13

4 references plus all compounds in the citations

FILE 'CAOLD' ENTERED AT 15:05:49 ON 22 JUN 1999

L15 0 S L8 AND L7

FILE 'BEILSTEIN' ENTERED AT 15:06:00 ON 22 JUN 1999

L16 STR L3
L17 42 S L16 FUL
L18 STR L16
L19 42 S L18 FUL
L20 STR L18
L21 42 S L20 FUL
L22 42 S L21 AND PRE/FA
L23 24 S FUJISHIMA, TOSHIE?/AU AND LIU, ZHAOPENG?/AU AND MIURA,

I printed 4 references.

42 compounds were contained in 4 different References

DAISHI

L24 26 S L22 NOT L23
L25 98 S KONNO, KATSUHIRO?/AU AND MAKI, SHOJIRO?/AU AND FUJISHIMA,
TOS

L26 98 S L25 AND 1998/PY

L27 10 S L24 NOT L26

L28 25 S ONO, YOSHIYUKI?/AU AND WATANABE, HIROYOSHI?/AU AND

SHIRAISHI,

L29 25 S L28 AND 1997/PY

L30 5 S L27 NOT L29

L31 55 S POSNER, GARY H?/AU AND CHO, CHEON-GYU?/AU AND ANJEH, TIZAH
E.

L32 55 S L31 AND 1995/PY

L33 0 S L30 NOT L32

FILE 'USPATFULL' ENTERED AT 15:15:15 ON 22 JUN 1999
L34 1 S L8
L35 0 S L34 AND L7

← Ø hits US Pat file

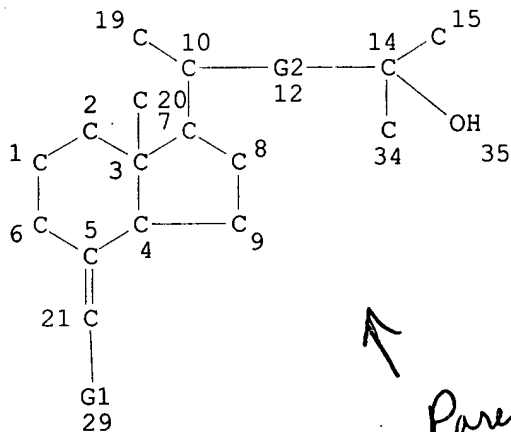
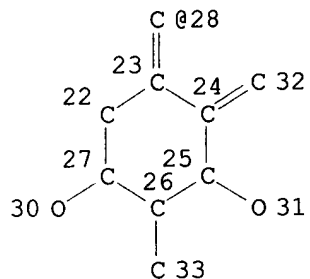
FILE 'CASREACT' ENTERED AT 15:15:37 ON 22 JUN 1999
L36 3 S L8
L37 5 S L7
L38 1 S L36 AND L37

← 1 reaction Casreact

=> d que 17

L3

STR



↑
Parent Search covers
Product and reactant.

VAR G1=X/28

REP G2=(0-9) CH2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

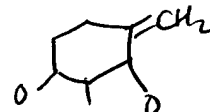
L5 36 SEA FILE=REGISTRY SSS FUL L3

L7 2 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT 46.150.1/RID

↑

Reactant.

← This gets rid of



=> d bib abs hitstr

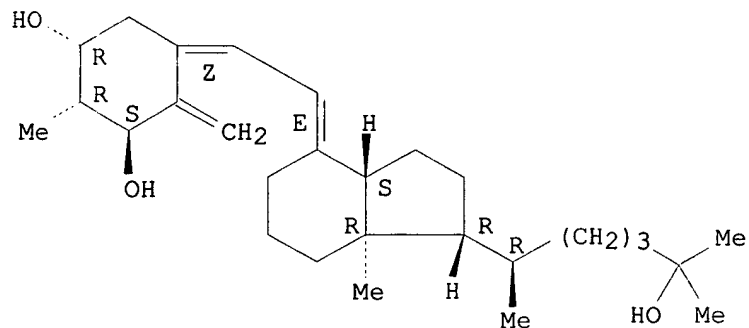
L14 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 1999 ACS
AN 1999:271054 HCAPLUS
DN 130:296894
TI Preparation of vitamin D3 derivatives for the treatment of osteoporosis
IN Takayama, Hiroaki; Konno, Katsuhiko; Maki, Shojiro
PA Teijin Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 24 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 11116551	A2	19990427	JP 98-160647	19970502
PRAI	JP 96-235144		19960905		
	JP 96-314693		19961126		
	JP 97-114695		19970502		
OS	MARPAT 130:296894				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 1,25-Dihydroxy-2-methylvitamin D3 derivs. of formula I [R1, R2 = H, alkyl]
are prepd. for the treatment of osteoporosis. Thus, III was added to IV, then deprotected to give II. The vitamin D receptor affinity of II was 400, compared to 100 for 1.alpha.,25-dihydroxyvitamin D3.
IT 158388-11-5P 203126-73-2P 203126-91-4P
203126-92-5P 203126-93-6P 203126-94-7P
203126-95-8P 203126-96-9P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of vitamin D3 derivs. for the treatment of osteoporosis)
RN 158388-11-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

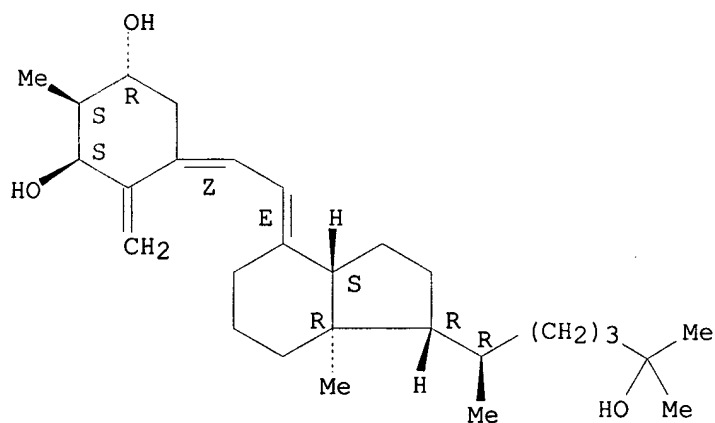


RN 203126-73-2 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

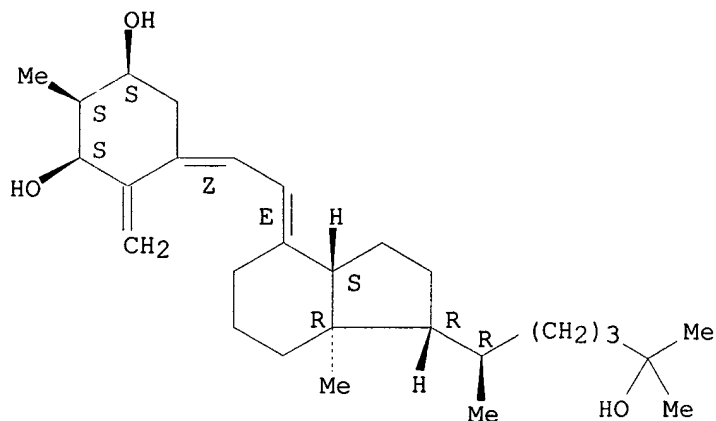


RN 203126-91-4 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

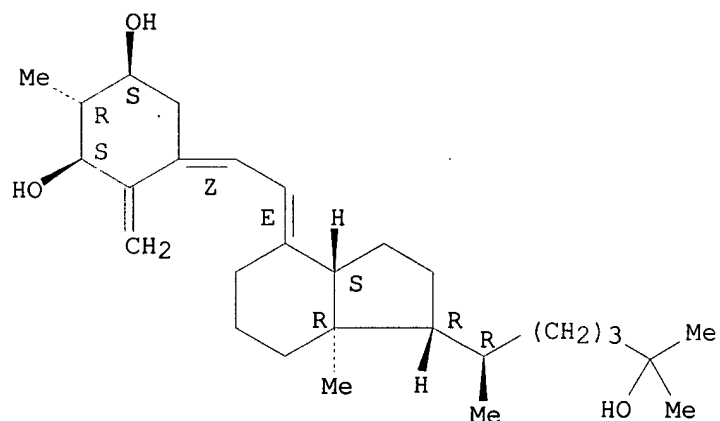


RN 203126-92-5 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

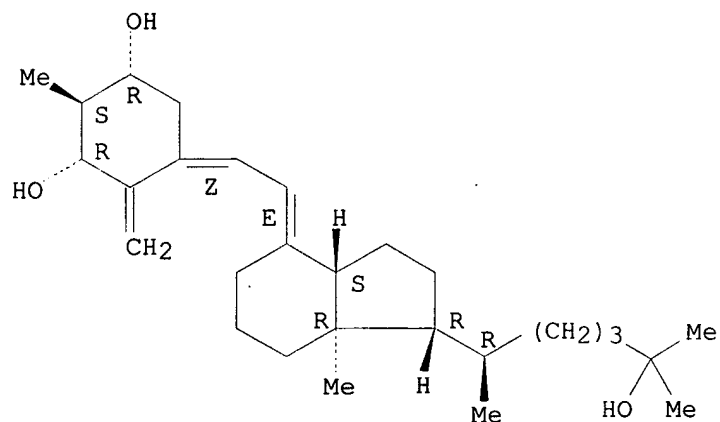


RN 203126-93-6 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.beta.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

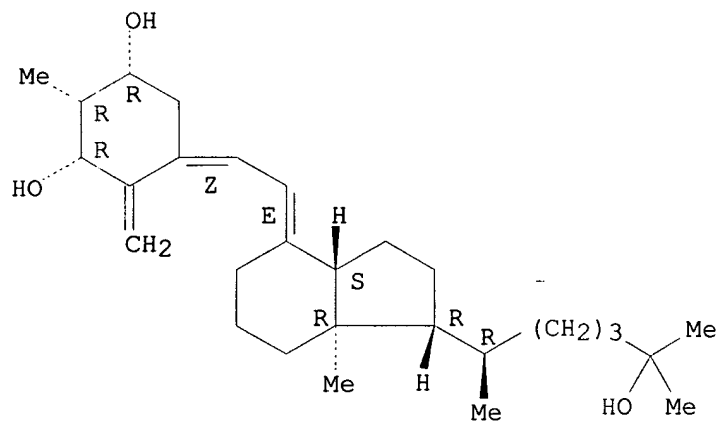
Double bond geometry as shown.



RN 203126-94-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.β.,5Z,7E)- (9CI) (CA INDEX NAME)

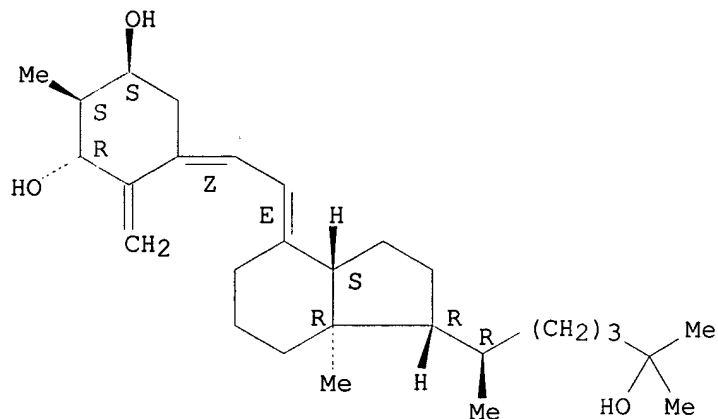
Absolute stereochemistry.
Double bond geometry as shown.



RN 203126-95-8 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.α.,3.α.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

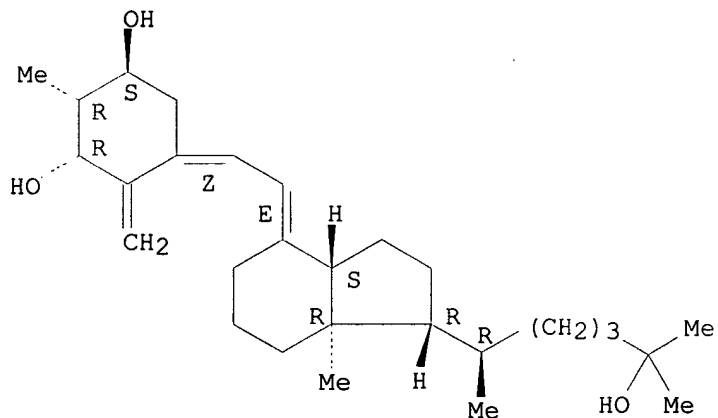


RN 203126-96-9 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.α.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



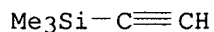
IT 1066-54-2, Ethynyltrimethylsilane 20445-33-4,
(S)-MTPA-Cl 39637-99-5, (R)-MTPA-Cl 80657-57-4
143705-63-9

RL: RCT (Reactant)

(prepn. of vitamin D3 derivs. for the treatment of osteoporosis)

RN 1066-54-2 HCAPLUS

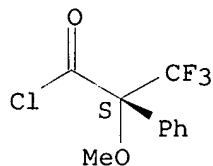
CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 20445-33-4 HCAPLUS

CN Benzeneacetyl chloride, .α.-methoxy-.α.-(trifluoromethyl)-,
(.α.S)- (9CI) (CA INDEX NAME).

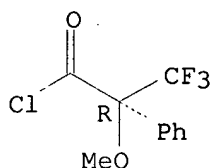
Absolute stereochemistry. Rotation (+).



RN 39637-99-5 HCAPLUS

CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (.alpha.R)- (9CI) (CA INDEX NAME)

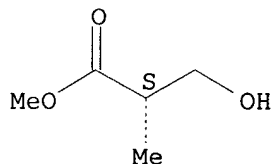
Absolute stereochemistry. Rotation (-).



RN 80657-57-4 HCAPLUS

CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

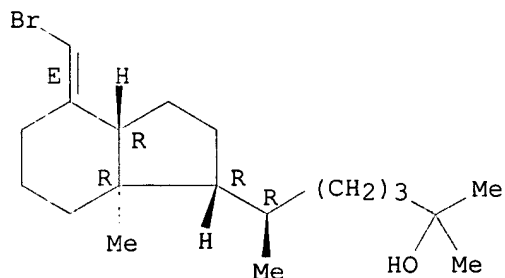
Absolute stereochemistry. Rotation (+).



RN 143705-63-9 HCAPLUS

CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 92817-88-4P 95514-03-7P 95514-04-8P
132117-93-2P 203126-90-3P 215394-09-5P

215394-10-8P 215394-12-0P 215394-15-3P
215394-17-5P 215394-20-0P 215394-22-2P
215394-23-3P 215394-24-4P 215394-34-6P
215394-35-7P 215394-36-8P 223437-33-0P
223437-37-4P 223437-39-6P 223437-51-2P
223437-60-3P

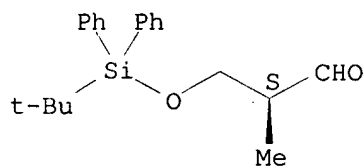
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of vitamin D3 derivs. for the treatment of osteoporosis)

RN 92817-88-4 HCAPLUS

CN Propanal, 3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-, (2S)-
(9CI)

(CA INDEX NAME)

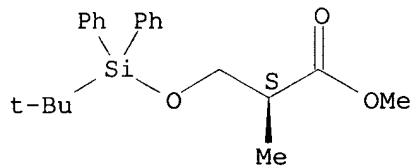
Absolute stereochemistry. Rotation (+).



RN 95514-03-7 HCAPLUS

CN Propanoic acid, 3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-,
methyl ester, (2S)- (9CI) (CA INDEX NAME)

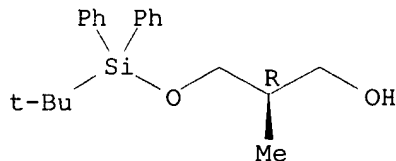
Absolute stereochemistry. Rotation (+).



RN 95514-04-8 HCAPLUS

CN 1-Propanol, 3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-, (2R)-
(9CI) (CA INDEX NAME)

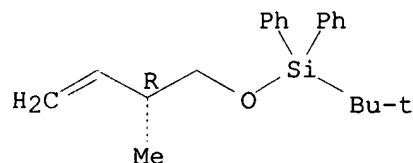
Absolute stereochemistry. Rotation (+).



RN 132117-93-2 HCAPLUS

CN Silane, (1,1-dimethylethyl)[[(2R)-2-methyl-3-butenyl]oxy]diphenyl- (9CI)
(CA INDEX NAME)

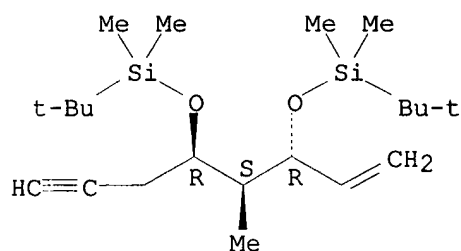
Absolute stereochemistry.



RN 203126-90-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

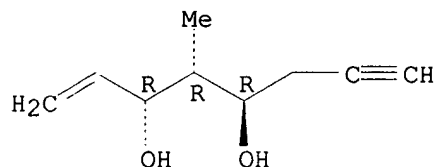
Absolute stereochemistry. Rotation (+).



RN 215394-09-5 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3R,4R,5R)- (9CI) (CA INDEX NAME)

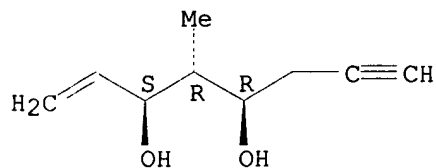
Absolute stereochemistry.



RN 215394-10-8 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3S,4R,5R)- (9CI) (CA INDEX NAME)

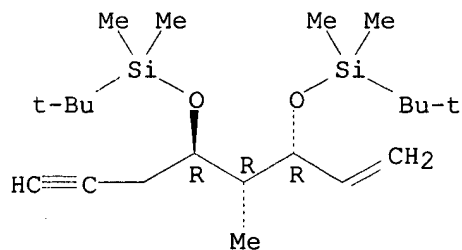
Absolute stereochemistry.



RN 215394-12-0 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7R)- (9CI) (CA INDEX NAME)

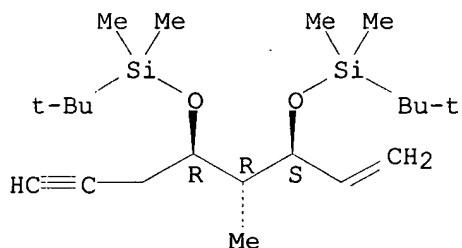
Absolute stereochemistry.



RN 215394-15-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7R)- (9CI) (CA INDEX NAME)

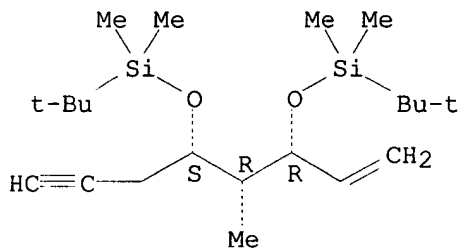
Absolute stereochemistry.



RN 215394-17-5 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7S)- (9CI) (CA INDEX NAME)

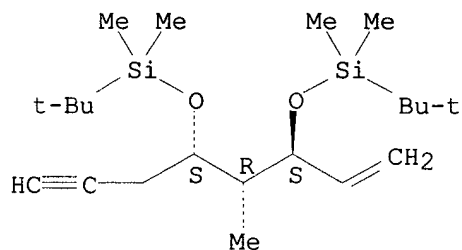
Absolute stereochemistry.



RN 215394-20-0 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7S)- (9CI) (CA INDEX NAME)

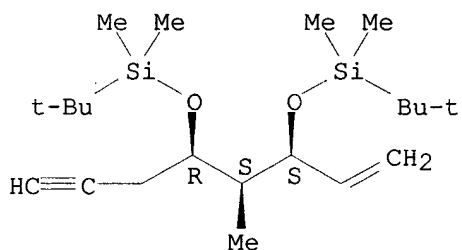
Absolute stereochemistry.



RN 215394-22-2 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethynyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7R)- (9CI) (CA INDEX NAME)

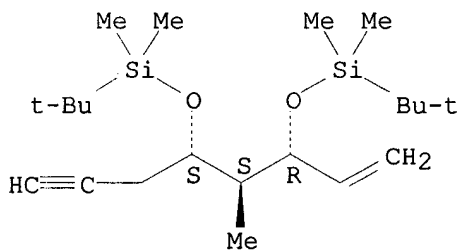
Absolute stereochemistry.



RN 215394-23-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethynyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7S)- (9CI) (CA INDEX NAME)

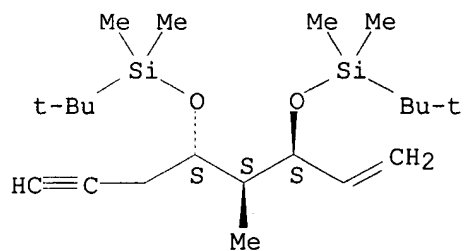
Absolute stereochemistry.



RN 215394-24-4 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethynyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7S)- (9CI) (CA INDEX NAME)

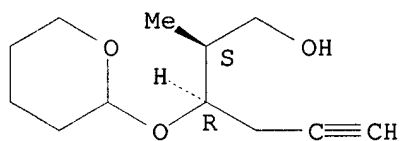
Absolute stereochemistry.



RN 215394-34-6 HCAPLUS

CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2S,3R)- (9CI)
(CA INDEX NAME)

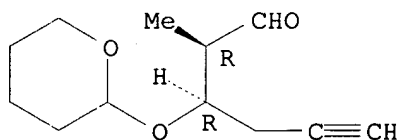
Absolute stereochemistry.



RN 215394-35-7 HCAPLUS

CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2R,3R)- (9CI)
(CA INDEX NAME)

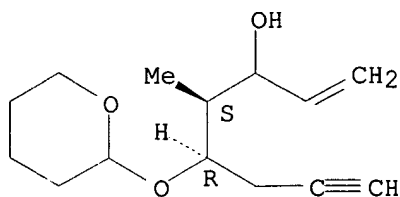
Absolute stereochemistry.



RN 215394-36-8 HCAPLUS

CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, (4S,5R)-
(9CI) (CA INDEX NAME)

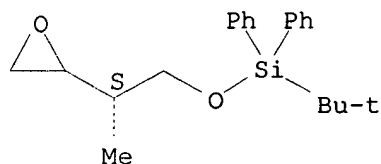
Absolute stereochemistry.



RN 223437-33-0 HCAPLUS

CN Silane, (1,1-dimethylethyl)[(2S)-2-oxiranylpropoxy]diphenyl- (9CI) (CA
INDEX NAME)

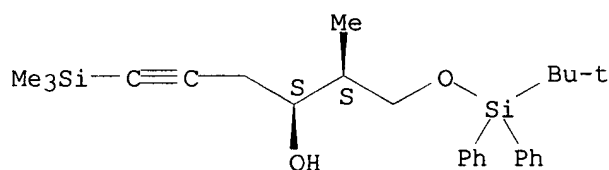
Absolute stereochemistry.



RN 223437-37-4 HCAPLUS

CN 5-Hexyn-3-ol, 1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3S)- (9CI) (CA INDEX NAME)

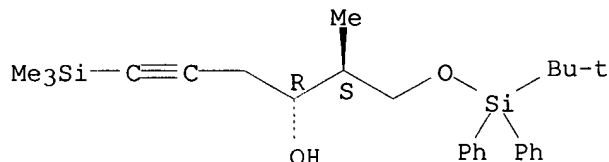
Absolute stereochemistry.



RN 223437-39-6 HCAPLUS

CN 5-Hexyn-3-ol, 1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3R)- (9CI) (CA INDEX NAME)

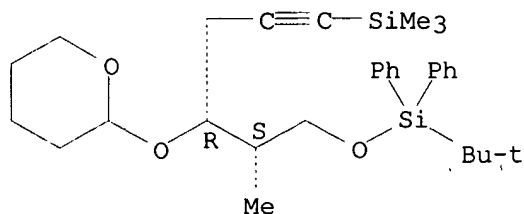
Absolute stereochemistry.



RN 223437-51-2 HCAPLUS

CN Silane, [(4R,5S)-6-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-5-methyl-4-[(tetrahydro-2H-pyran-2-yl)oxy]-1-hexynyl]trimethyl- (9CI) (CA INDEX NAME)

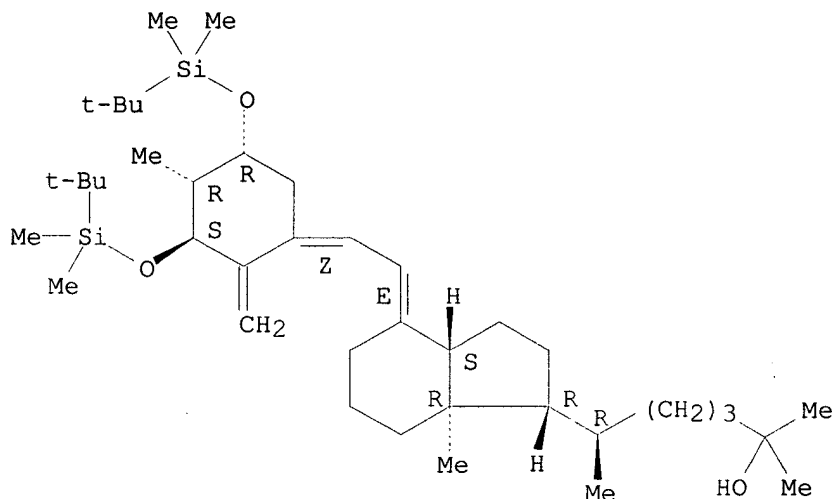
Absolute stereochemistry.



RN 223437-60-3 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-trien-25-ol, 1,3-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



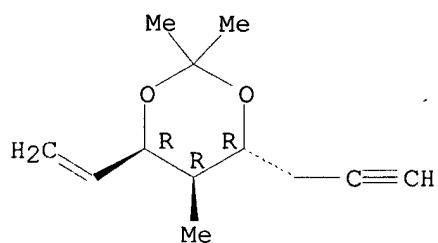
IT 215394-37-9P 215394-38-0P 223437-41-0P
223437-43-2P 223437-46-5P 223437-49-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of vitamin D3 derivs. for the treatment of osteoporosis)

RN 215394-37-9 HCAPLUS

CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4R,5R,6R)- (9CI)
(CA INDEX NAME)

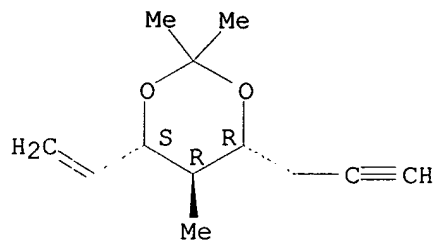
Absolute stereochemistry.



RN 215394-38-0 HCAPLUS

CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4S,5R,6R)- (9CI)
(CA INDEX NAME)

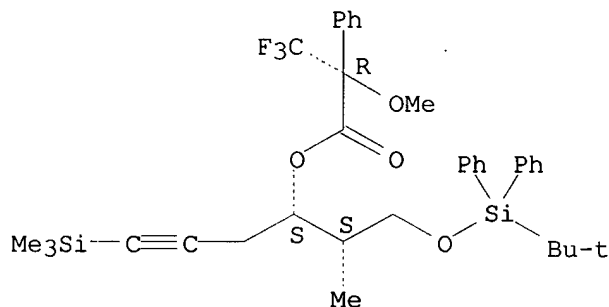
Absolute stereochemistry.



RN 223437-41-0 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

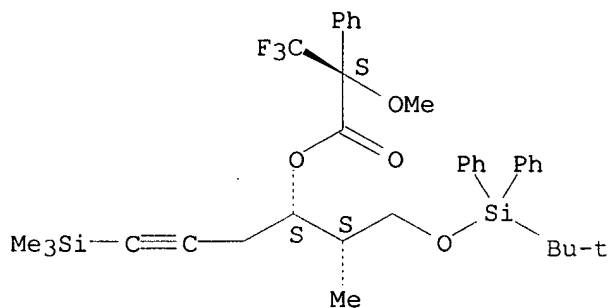
Absolute stereochemistry.



RN 223437-43-2 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

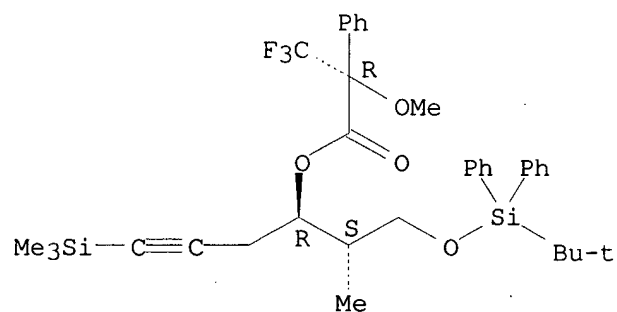
Absolute stereochemistry.



RN 223437-46-5 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

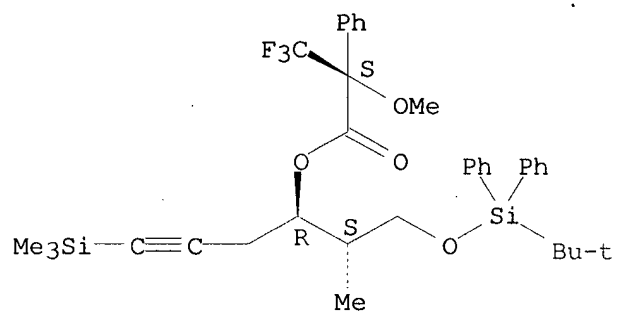
Absolute stereochemistry.



RN 223437-49-8 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-,
(1R)-1-[(1S)-2-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1-methylethyl]-4-
(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d bib abs hitstr 2

L14 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 1999 ACS

AN 1998:745027 HCAPLUS

DN 129:343629

TI Preparation of vitamin D3 derivatives and their pharmaceutical uses

IN Takayama, Hiroaki; Konno, Katsuhiko; Fujishima, Toshie

PA Teijin Ltd., Japan

SO PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9850353	A1	19981112	WO 98-JP1979	19980430
	W: JP, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI	JP 97-114695		19970502		
OS	CASREACT 129:343629; MARPAT 129:343629				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 1,25-Dihydroxy-2-Me vitamin D3 derivs. I [R1, R2 = H, tri(C1-7alkyl)silyl;

the asym. carbon atoms at the 1-, 2- and 3-positions each independently has an .alpha.- or .beta.-configuration], useful as remedies for osteoporosis, rachitis, accessory thyroidal hyperenergia, etc., are prepd.

via reaction of II (X = bromo, iodo) with III (R3, R4 = H, trihydrocarbylsilyl) in the presence of a palladium catalyst optionally followed by deprotection (removal of silyl groups). Thus, II (X = Br) was

reacted with III (R3 = R4 = TBS) in toluene contg. Et3N, Pd2(dba)3.CHCl3, and Ph3P at 120.degree. to give IV (R = TBS), which was treated with camphor-10-sulfonic acid in methanol to give 63% IV (R = H). In a study using 1.alpha.,25-dihydroxyvitamin D3 receptors in the bovine thymus gland, this showed an affinity of 160 compared with 100 for 1.alpha.,25-dihydroxyvitamin D3.

IT 158388-11-5P 214351-93-6P 214351-94-7P

214351-95-8P 214351-96-9P 214351-97-0P

214351-98-1P 214351-99-2P 215394-65-3P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

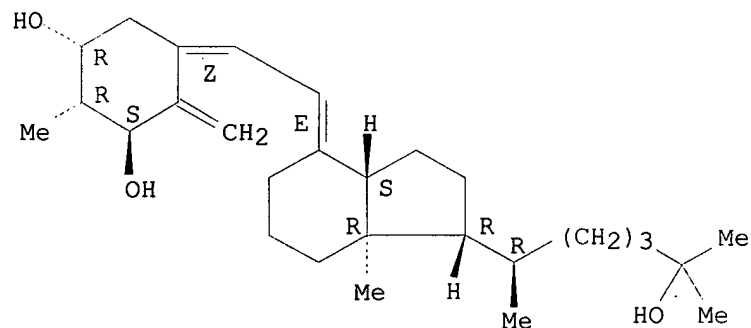
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)

RN 158388-11-5 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

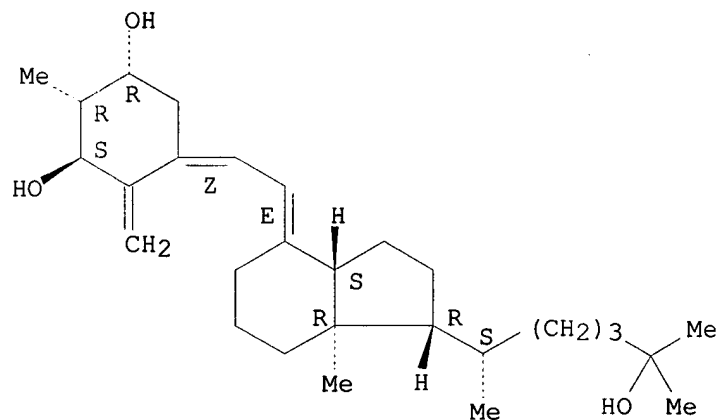
Double bond geometry as shown.



RN 214351-93-6 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

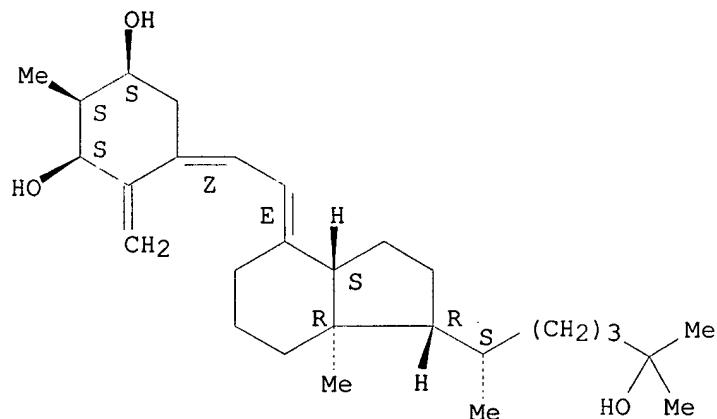
Absolute stereochemistry.
Double bond geometry as shown.



RN 214351-94-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

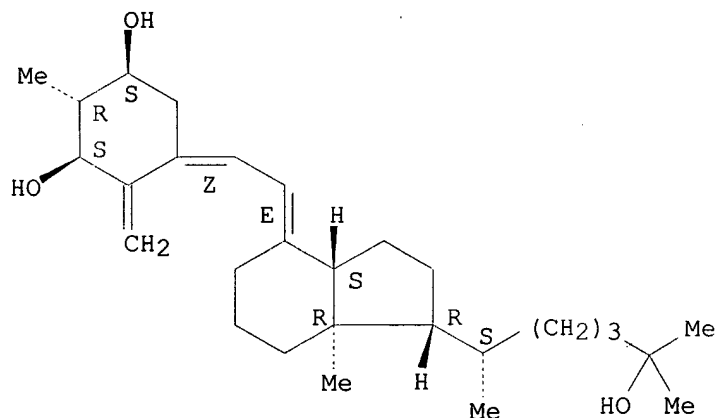


RN 214351-95-8 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

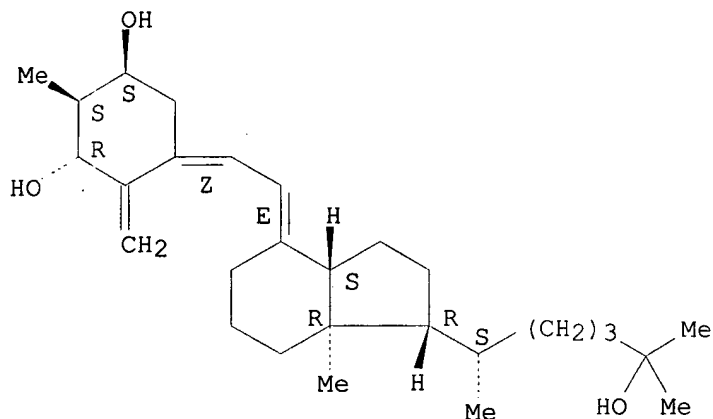


RN 214351-96-9 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.beta.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

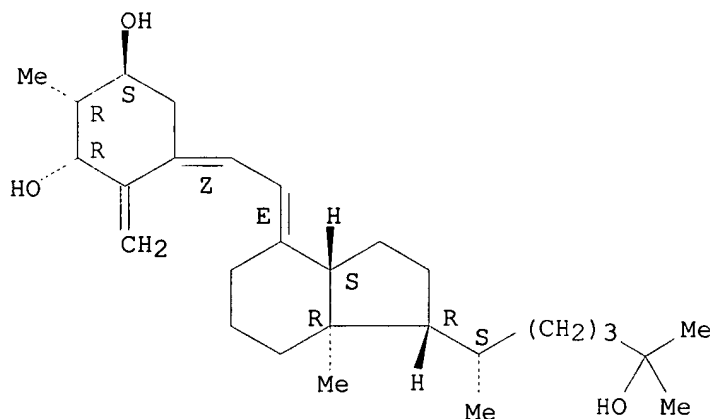


RN 214351-97-0 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.α.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

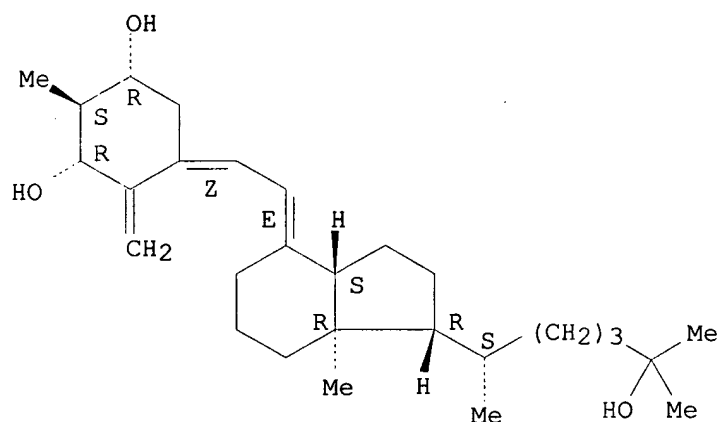


RN 214351-98-1 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.α.,3.β.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

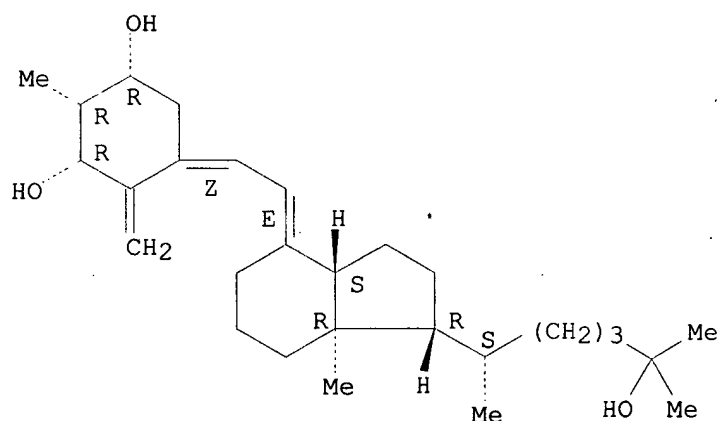


RN 214351-99-2 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.beta.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

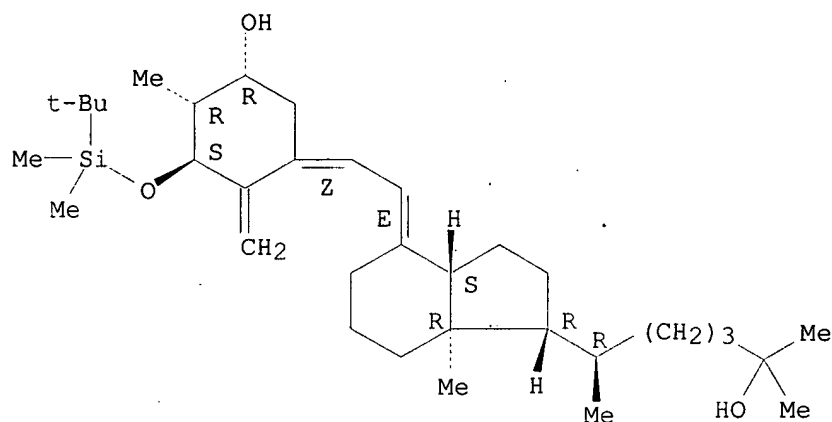


RN 215394-65-3 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-3,25-triol, 1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-,
(1.alpha.,2.beta.,3.beta.,5Z,7
E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 52522-40-4

RL: CAT (Catalyst use); USES (Uses)

(prepn. of vitamin D3 derivs. and their pharmaceutical uses)

RN 52522-40-4 HCAPLUS

CN Palladium, tris[.mu.-[(1,2-.eta.:4,5-.eta.)-(1E,4E)-1,5-diphenyl-1,4-pentadien-3-one]]di-, compd. with trichloromethane (1:1) (9CI) (CA INDEX NAME)

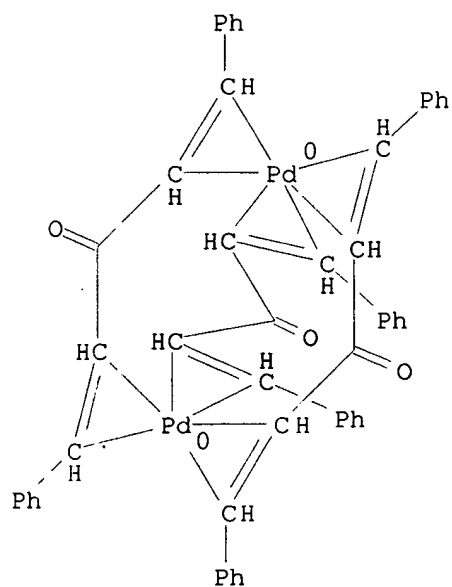
CM 1

CRN 51364-51-3

CMF C51 H42 O3 Pd2

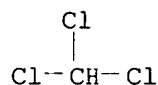
CCI CCS

CDES 2:ALL,E

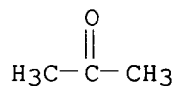


CM 2

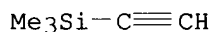
CRN 67-66-3
CMF C H Cl3



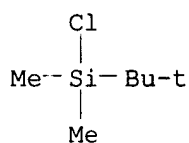
IT 67-64-1, 2-Propanone, reactions 1066-54-2,
Ethynyltrimethylsilane 18162-48-6, tert-Butyldimethylsilyl
chloride 20445-33-4 39637-99-5 69739-34-0,
tert-Butyldimethylsilyl triflate 143705-63-9 214351-89-0
RL: RCT (Reactant)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)
RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)



RN 1066-54-2 HCAPLUS
CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

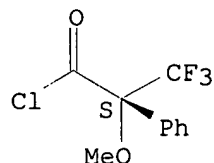


RN 18162-48-6 HCAPLUS
CN Silane, chloro(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



RN 20445-33-4 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-,
(.alpha.S)- (9CI) (CA INDEX NAME)

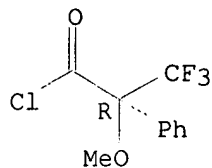
Absolute stereochemistry. Rotation (+).



RN 39637-99-5 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-,

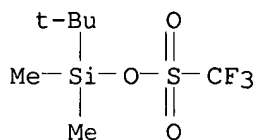
(.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 69739-34-0 HCAPLUS

CN Methanesulfonic acid, trifluoro-, (1,1-dimethylethyl)dimethylsilyl ester
(9CI) (CA INDEX NAME)

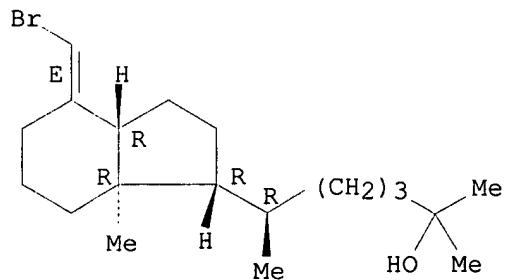


RN 143705-63-9 HCAPLUS

CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-
.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

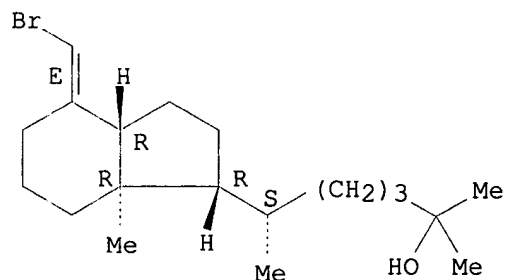


RN 214351-89-0 HCAPLUS

CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-
.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4E,7aR)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 104701-87-3P 112057-64-4P 147915-53-5P
 147915-54-6P 203126-90-3P 215394-09-5P
 215394-10-8P 215394-12-0P 215394-15-3P
 215394-17-5P 215394-20-0P 215394-22-2P
 215394-23-3P 215394-24-4P 215394-25-5P
 215394-26-6P 215394-27-7P 215394-28-8P
 215394-29-9P 215394-30-2P 215394-31-3P
 215394-32-4P 215394-33-5P 215394-34-6P
 215394-35-7P 215394-36-8P 215394-37-9P
 215394-38-0P

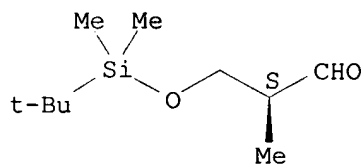
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of vitamin D3 derivs. and their pharmaceutical uses)

RN 104701-87-3 HCAPLUS

CN Propanal, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (2S)-
 (9CI)

(CA INDEX NAME)

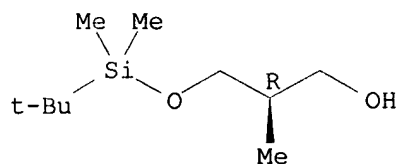
Absolute stereochemistry.



RN 112057-64-4 HCAPLUS

CN 1-Propanol, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (2R)-
 (9CI) (CA INDEX NAME)

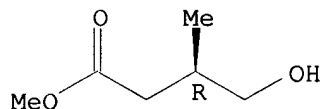
Absolute stereochemistry. Rotation (+).



RN 147915-53-5 HCAPLUS

CN Butanoic acid, 4-hydroxy-3-methyl-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

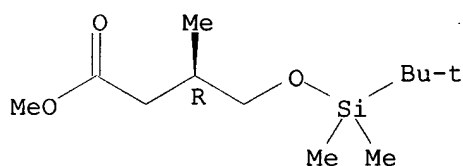
Absolute stereochemistry.



RN 147915-54-6 HCAPLUS

CN Butanoic acid, 4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-methyl-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

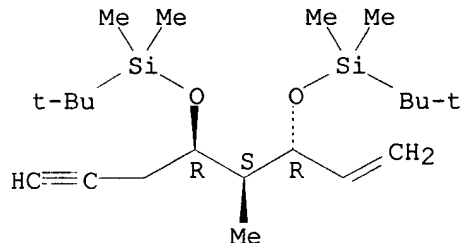
Absolute stereochemistry.



RN 203126-90-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

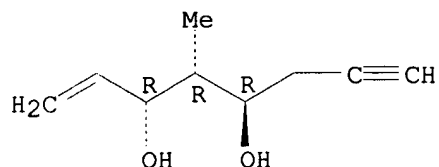
Absolute stereochemistry. Rotation (+).



RN 215394-09-5 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3R,4R,5R)- (9CI) (CA INDEX NAME)

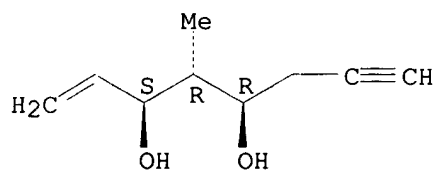
Absolute stereochemistry.



RN 215394-10-8 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3S,4R,5R)- (9CI) (CA INDEX NAME)

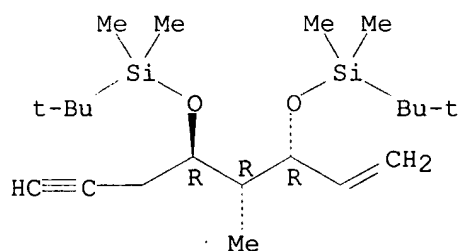
Absolute stereochemistry.



RN 215394-12-0 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7R)- (9CI) (CA INDEX NAME)

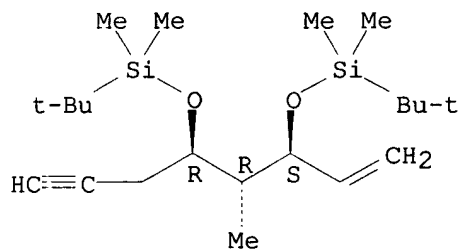
Absolute stereochemistry.



RN 215394-15-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7R)- (9CI) (CA INDEX NAME)

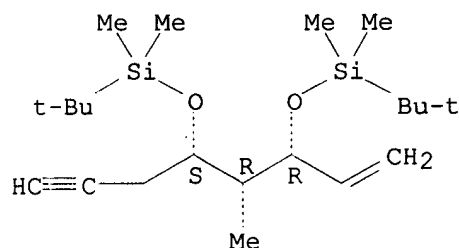
Absolute stereochemistry.



RN 215394-17-5 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7S)- (9CI) (CA INDEX NAME)

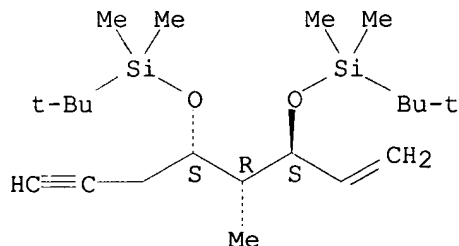
Absolute stereochemistry.



RN 215394-20-0 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7S)- (9CI) (CA INDEX NAME)

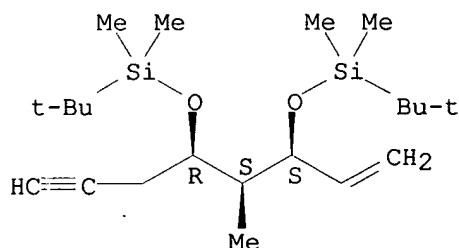
Absolute stereochemistry.



RN 215394-22-2 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7R)- (9CI) (CA INDEX NAME)

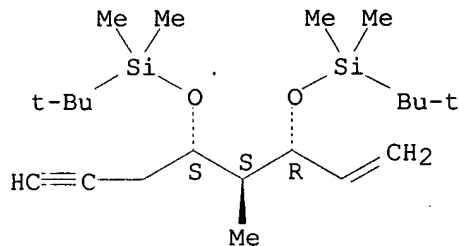
Absolute stereochemistry.



RN 215394-23-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7S)- (9CI) (CA INDEX NAME)

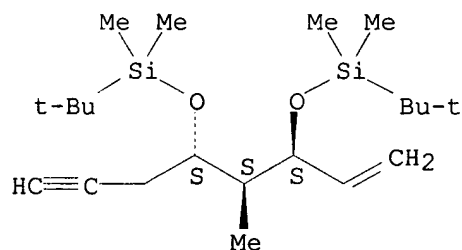
Absolute stereochemistry.



RN 215394-24-4 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7S)- (9CI) (CA INDEX NAME)

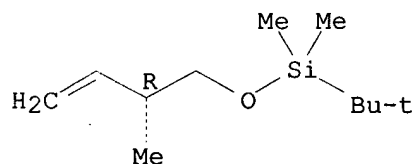
Absolute stereochemistry.



RN 215394-25-5 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[[(2R)-2-methyl-3-butenyl]oxy]- (9CI)
(CA INDEX NAME)

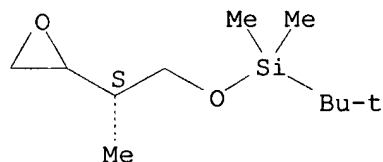
Absolute stereochemistry.



RN 215394-26-6 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[(2S)-2-oxiranylpropoxy]- (9CI) (CA INDEX NAME)

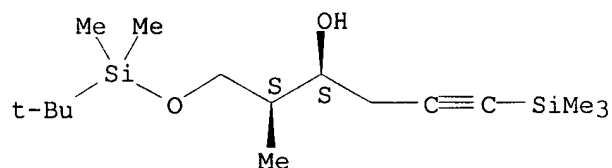
Absolute stereochemistry.



RN 215394-27-7 HCAPLUS

CN 5-Hexyn-3-ol, 1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3S)- (9CI) (CA INDEX NAME)

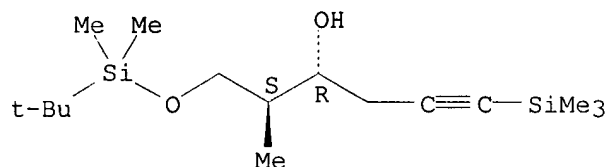
Absolute stereochemistry.



RN 215394-28-8 HCAPLUS

CN 5-Hexyn-3-ol, 1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3R)- (9CI) (CA INDEX NAME)

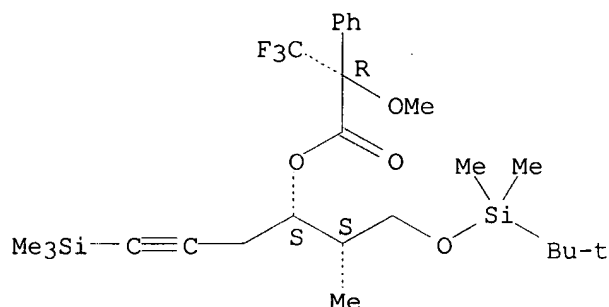
Absolute stereochemistry.



RN 215394-29-9 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

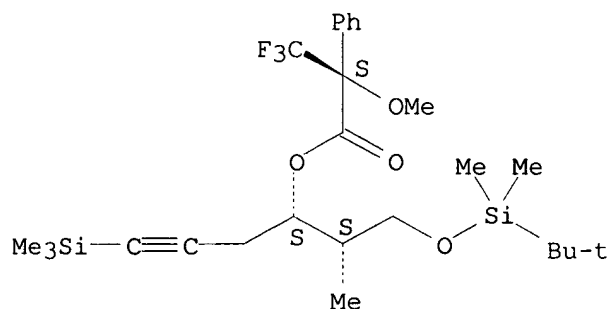
Absolute stereochemistry.



RN 215394-30-2 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

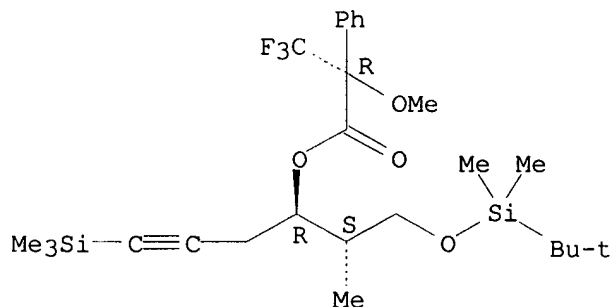
Absolute stereochemistry.



RN 215394-31-3 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

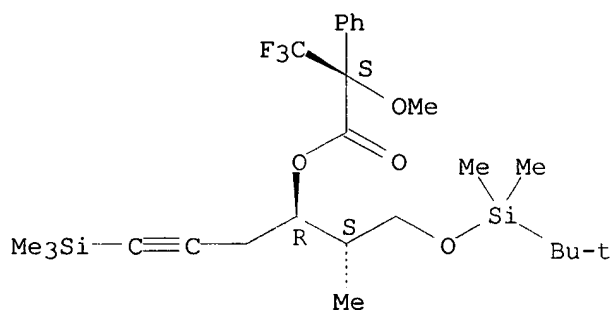
Absolute stereochemistry.



RN 215394-32-4 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-,
(1R)-1-[(1S)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-
(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

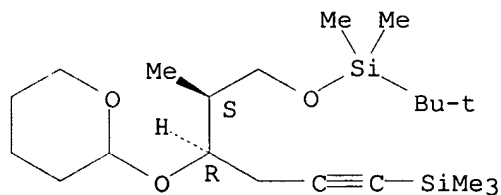
Absolute stereochemistry.



RN 215394-33-5 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[(2S,3R)-2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-3-[3-(trimethylsilyl)-2-propynyl]propoxy]- (9CI) (CA INDEX NAME)

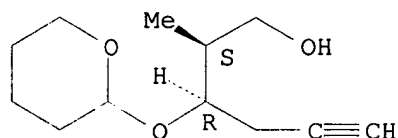
Absolute stereochemistry.



RN 215394-34-6 HCAPLUS

CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2S,3R)- (9CI)
(CA INDEX NAME)

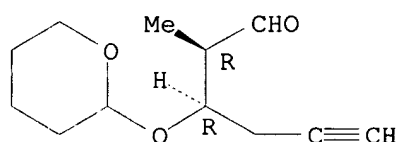
Absolute stereochemistry.



RN 215394-35-7 HCAPLUS

CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2R,3R)- (9CI)
(CA INDEX NAME)

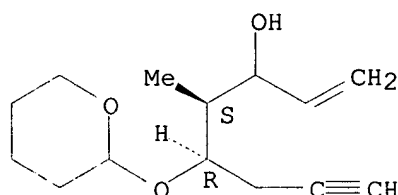
Absolute stereochemistry.



RN 215394-36-8 HCAPLUS

CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, (4S,5R)-
(9CI) (CA INDEX NAME)

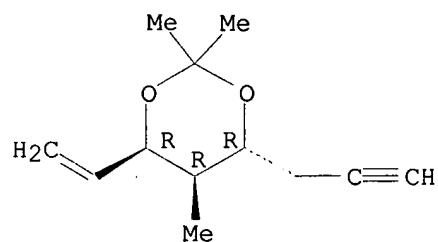
Absolute stereochemistry.



RN 215394-37-9 HCAPLUS

CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4R,5R,6R)- (9CI)
(CA INDEX NAME)

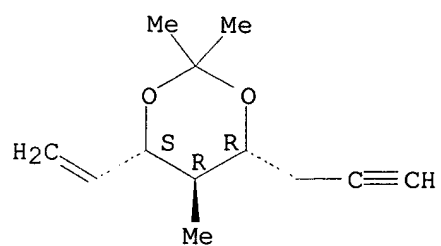
Absolute stereochemistry.



RN 215394-38-0 HCAPLUS

CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4S,5R,6R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



=> d bib abs hitstr 3

L14 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 1999 ACS

AN 1998:606883 HCAPLUS

DN 129:290279

TI Synthesis and biological activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3

AU Fujishima, Toshie; Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu; Ishizuka, Seiichi; Konno, Katsuhiro; Takayama, Hiroaki

CS Faculty of Pharmaceutical Sciences, Teikyo University, Kanagawa, 199-0195, Japan

SO Bioorg. Med. Chem. Lett. (1998), 8(16), 2145-2148

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

AB Synthesis and biol. evaluation of all eight possible A-ring diastereomers of 2-methyl-20-epi-1,25-dihydroxyvitamin D3 are described. Among the analogs synthesized, 2.alpha.-methyl-20-epi-1.alpha.,25-dihydroxyvitamin D3 exhibited exceptionally high potency. The double modification of 2-Me substitution and 20-epimerization yielded analogs with unique activity profiles.

IT 32222-06-3P, 1.alpha.,25-Dihydroxyvitamin D3

RL: PNU (Preparation, unclassified); PREP (Preparation)

(Synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)

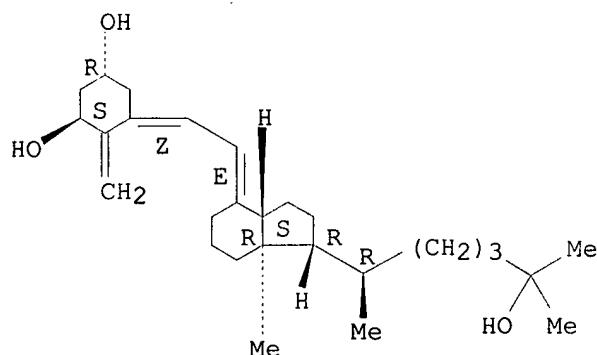
RN 32222-06-3 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.alpha.,3.beta.,5Z,7E)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 214351-84-5P 214351-93-6P 214351-94-7P

214351-95-8P 214351-96-9P 214351-97-0P

214351-98-1P 214351-99-2P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

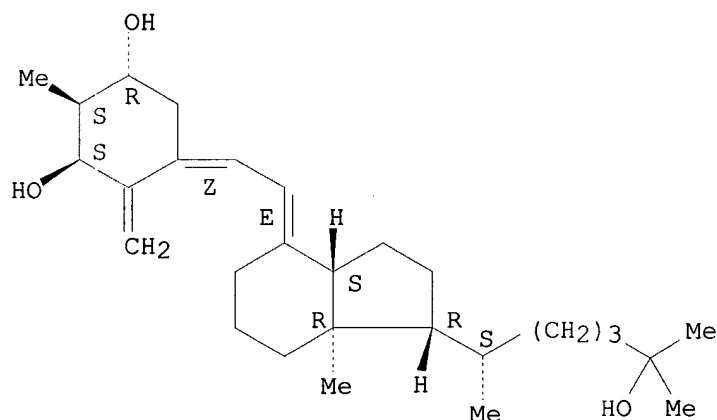
(synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)

RN 214351-84-5 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

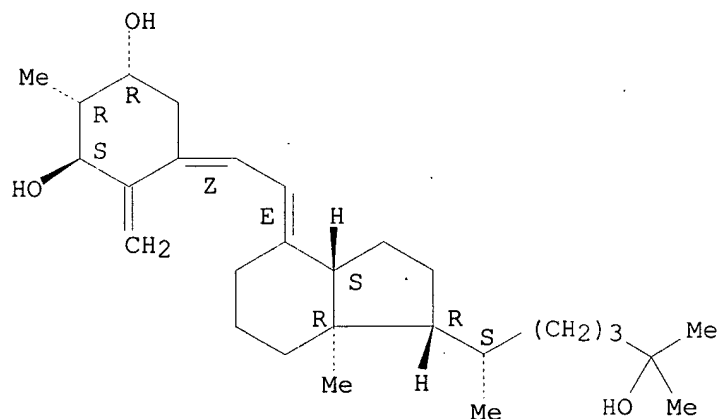


RN 214351-93-6 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

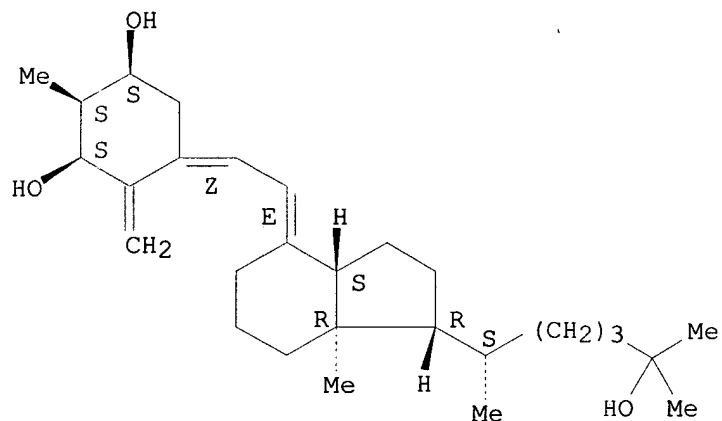


RN 214351-94-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

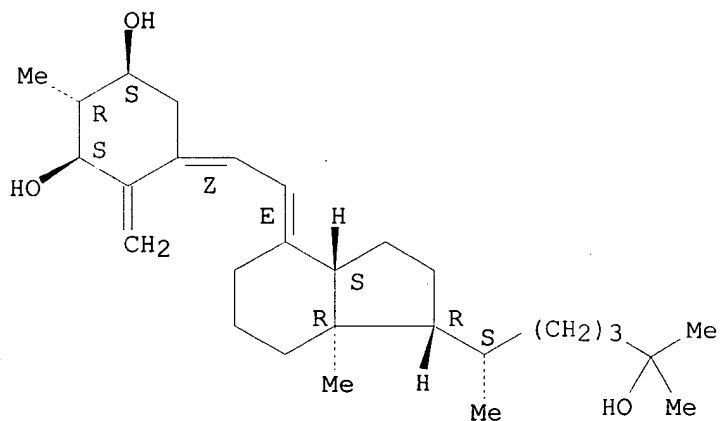


RN 214351-95-8 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

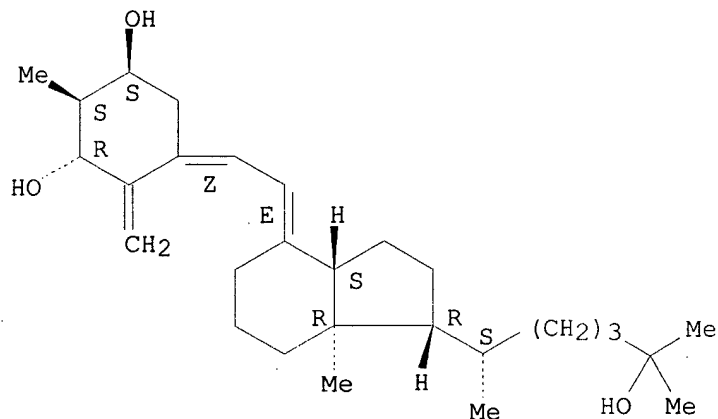


RN 214351-96-9 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.beta.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

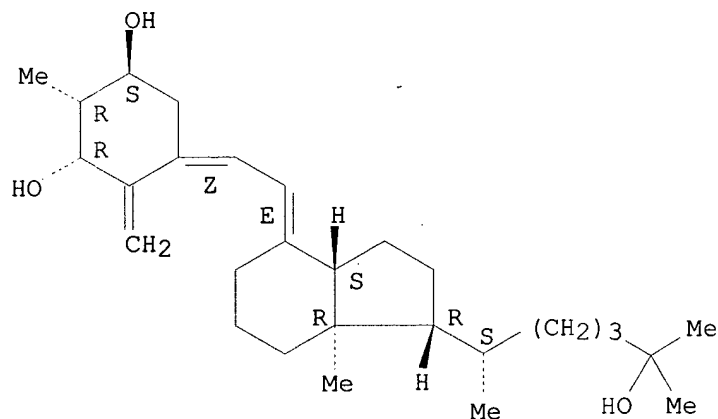


RN 214351-97-0 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.α.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

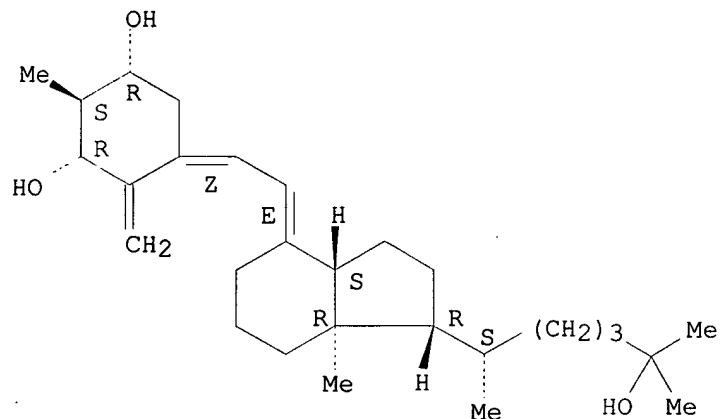


RN 214351-98-1 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.α.,3.β.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

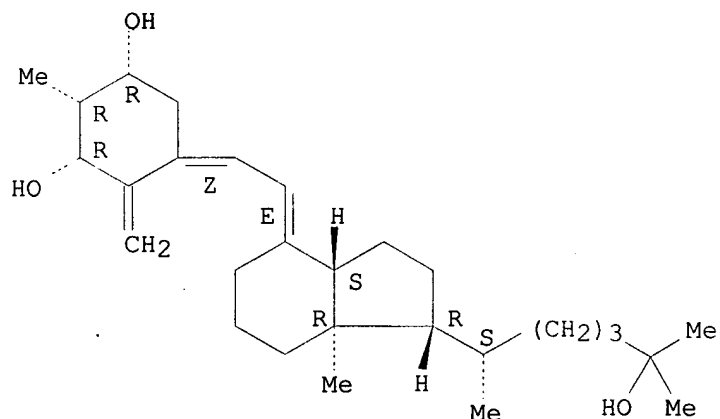


RN 214351-99-2 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.β.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 104651-47-0 203126-90-3 214351-87-8

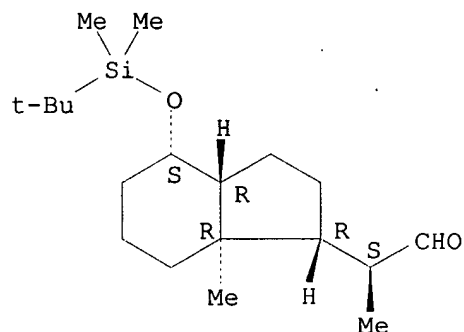
RL: RCT (Reactant)

(synthesis and biol. activity of 2-methyl-20-epi analogs of
1.α.,25-dihydroxyvitamin D3)

RN 104651-47-0 HCAPLUS

CN 1H-Indene-1-acetaldehyde,
4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahyd
ro-α.,7a-dimethyl-, (.α.S,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

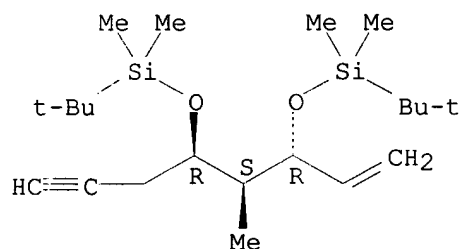
Absolute stereochemistry. Rotation (+).



RN 203126-90-3 HCAPLUS

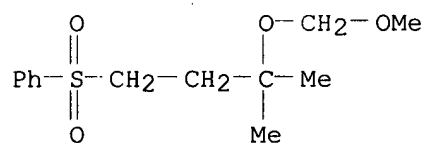
CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 214351-87-8 HCAPLUS

CN Benzene, [[3-(methoxymethoxy)-3-methylbutyl]sulfonyl]- (9CI) (CA INDEX NAME)



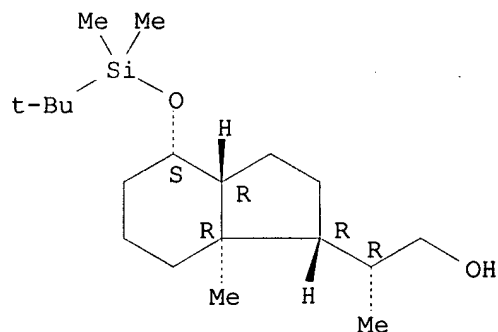
IT 171011-48-6P 183506-75-4P 213250-67-0P
214351-86-7P 214351-88-9P 214351-89-0P
214351-91-4P 214351-92-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and biol. activity of 2-methyl-20-epi analogs of
1.alpha.,25-dihydroxyvitamin D₃)

RN 171011-48-6 HCAPLUS

CN 1H-Indene-1-ethanol, 4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.beta.,7a-dimethyl-, (.beta.R,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

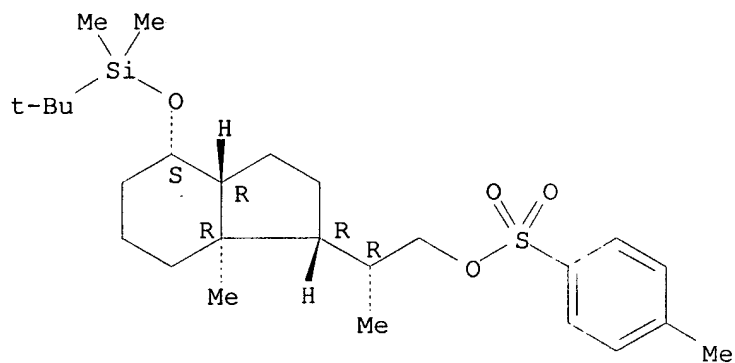
Absolute stereochemistry. Rotation (+).



RN 183506-75-4 HCAPLUS

CN 1H-Indene-1-ethanol, 4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.beta.,7a-dimethyl-, 4-methylbenzenesulfonate, (.beta.R,1R,3aR,4S,7aR)-(9CI) (CA INDEX NAME)

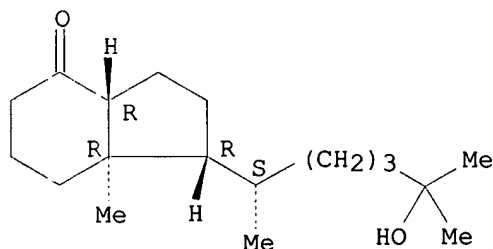
Absolute stereochemistry. Rotation (+).



RN 213250-67-0 HCAPLUS

CN 4H-Inden-4-one, octahydro-1-[(1S)-5-hydroxy-1,5-dimethylhexyl]-7a-methyl-, (1R,3aR,7aR)-(9CI) (CA INDEX NAME)

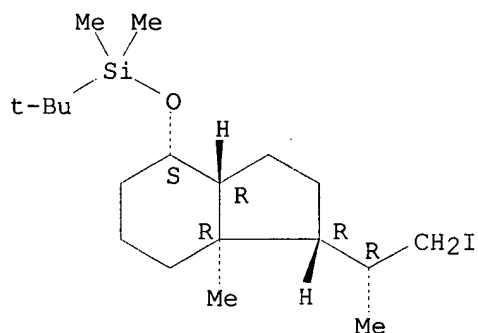
Absolute stereochemistry.



RN 214351-86-7 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[[[(1R,3aR,4S,7aR)-octahydro-1-[(1R)-2-iodo-1-methylethyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

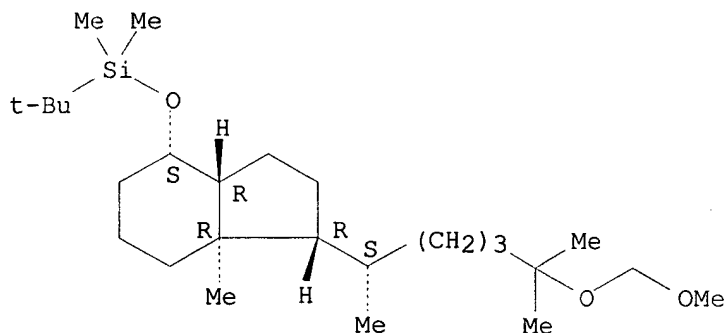
Absolute stereochemistry.



RN 214351-88-9 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[[(1R,3aR,4S,7aR)-octahydro-1-[(1S)-5-(methoxymethoxy)-1,5-dimethylhexyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

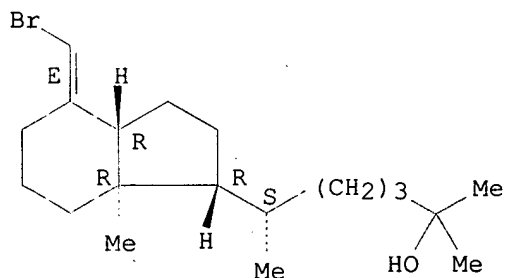


RN 214351-89-0 HCAPLUS

CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

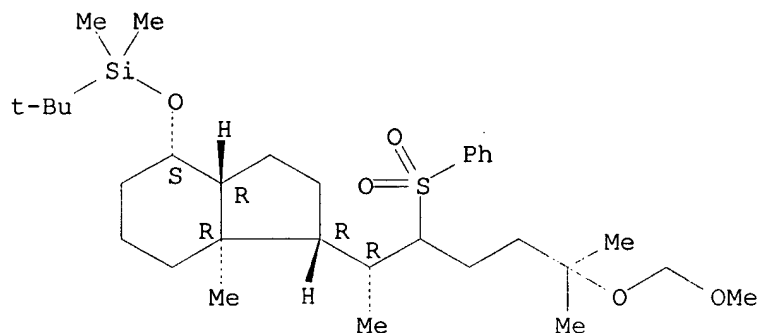


RN 214351-91-4 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[[(1R,3aR,4S,7aR)-octahydro-1-[(1R)-5-

(methoxymethoxy)-1,5-dimethyl-2-(phenylsulfonyl)hexyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

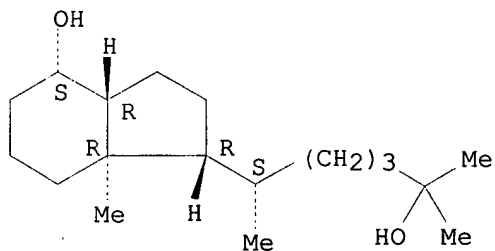
Absolute stereochemistry.



RN 214351-92-5 HCAPLUS

CN 1H-Indene-1-pentanol, octahydro-4-hydroxy-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d bib abs hitstr 4

L14 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 1999 ACS

AN 1998:85846 HCAPLUS

DN 128:180577

TI A novel and practical route to A-ring enyne synthon for
1.alpha.,25-dihydroxyvitamin D3 analogs: synthesis of A-ring
diastereomers

of 1.alpha.,25-dihydroxyvitamin D3 and 2-methyl-1,25-dihydroxyvitamin D3
AU Konno, Katsuhiko; Maki, Shojiro; Fujishima, Toshie; Liu, Zhaopeng; Miura,
Daishiro; Chokki, Manabu; Takayama, Hiroaki

CS Faculty Pharmaceutical Sciences, Teikyo Univ., Sagamiko, Kanagawa,
199-01,

Japan

SO Bioorg. Med. Chem. Lett. (1998), 8(2), 151-156

CODEN: BMCLE8; ISSN: 0960-894X

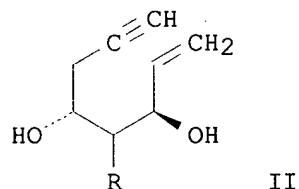
PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 128:180577

GI



AB A novel and practical route to the A-ring enyne synthon II (R = H, Me),
which can be versatile for a variety of A-ring analogs of
1.alpha.,25-dihydroxyvitamin D3 (I), was developed. This novel method
led

to an improved synthesis of the A-ring diastereomers of I, and synthesis
of the new analogs, 2-methyl-1,25-dihydroxyvitamin D3 with its all
possible diastereomers. The biol. evaluation of the 2-Me analogs showed
the .alpha..alpha..beta.-isomer to be more potent than I.

IT 32222-06-3DP, 1.alpha.,25-Dihydroxyvitamin D3, A-ring analogs

158388-11-5P 203126-73-2P 203126-91-4P

203126-92-5P 203126-93-6P 203126-94-7P

203126-95-8P 203126-96-9P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3
analog)

RN 32222-06-3 HCAPLUS

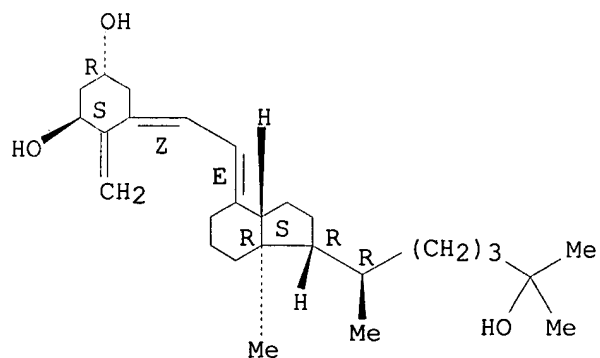
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol,

(1.alpha.,3.beta.,5Z,7E)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

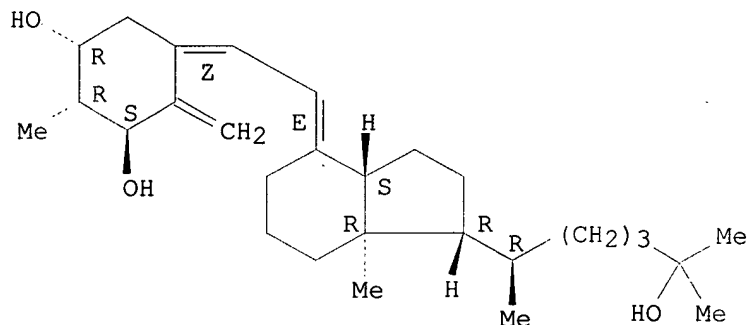
Double bond geometry as shown.



RN 158388-11-5 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

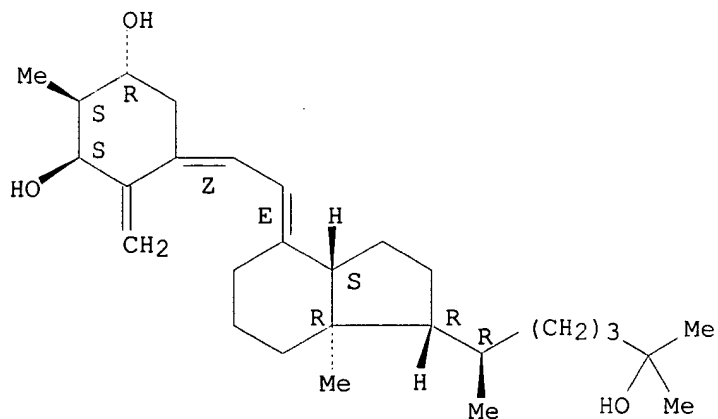
Absolute stereochemistry.
Double bond geometry as shown.



RN 203126-73-2 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

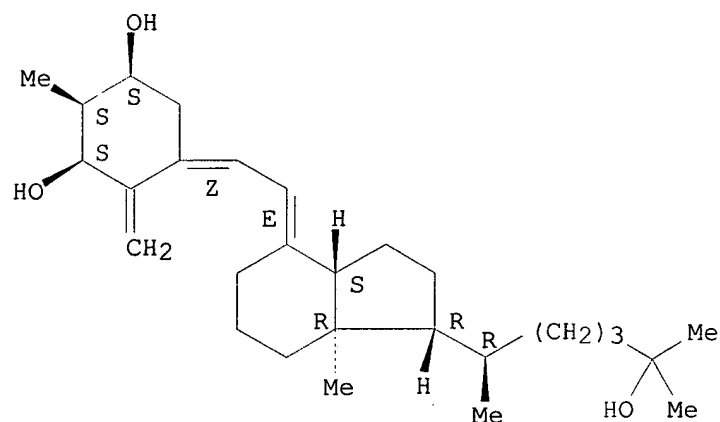


RN 203126-91-4 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

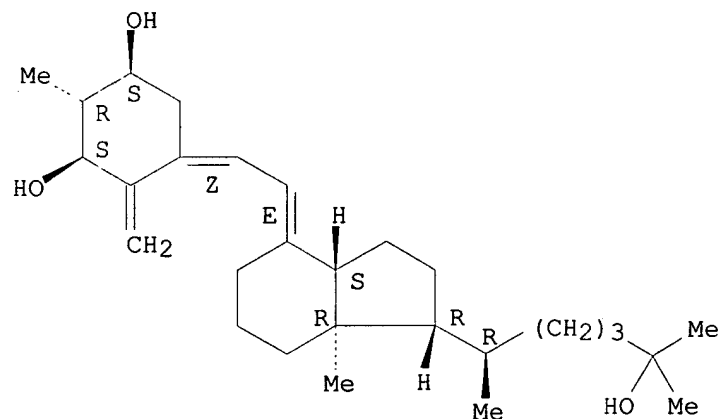


RN 203126-92-5 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

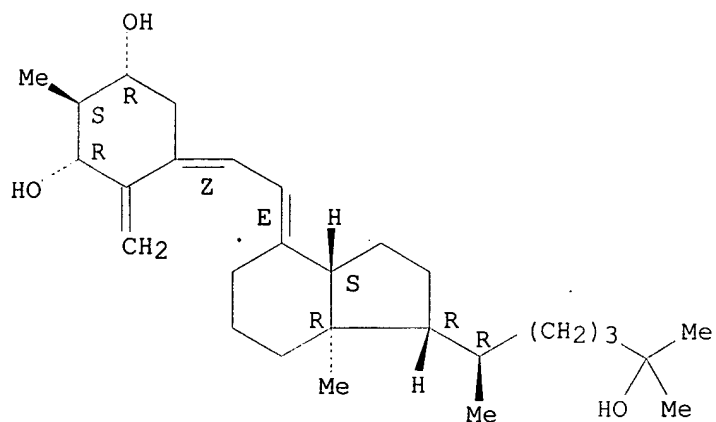


RN 203126-93-6 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.beta.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

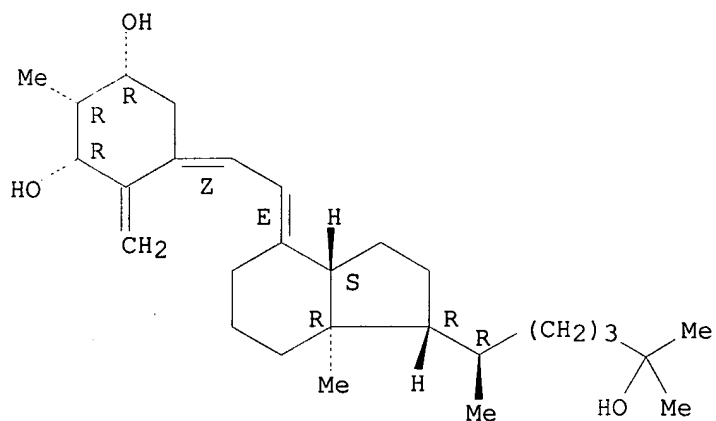


RN 203126-94-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.β.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

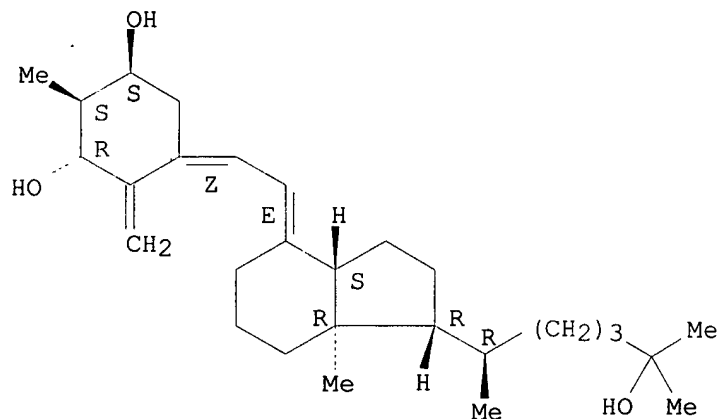


RN 203126-95-8 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.α.,3.α.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

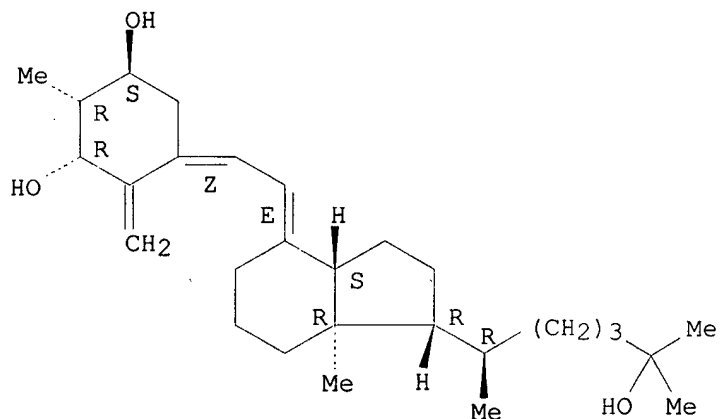


RN 203126-96-9 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.α.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



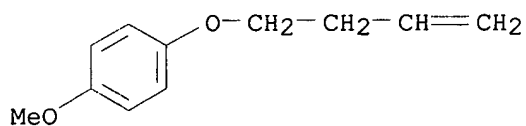
IT 2653-90-9 72657-23-9, Methyl (R)-3-hydroxy-2-methylpropionate 80657-57-4, Methyl (S)-3-hydroxy-2-methylpropionate 143705-63-9

RL: RCT (Reactant)

(prepn. of A-ring enyne synthons and 1.α.,25-dihydroxyvitamin D3 analogs)

RN 2653-90-9 HCAPLUS

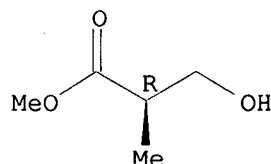
CN Benzene, 1-(3-butenyloxy)-4-methoxy- (7CI, 9CI) (CA INDEX NAME)



RN 72657-23-9 HCAPLUS

CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

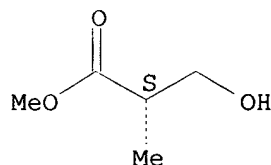
Absolute stereochemistry. Rotation (-).



RN 80657-57-4 HCAPLUS

CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

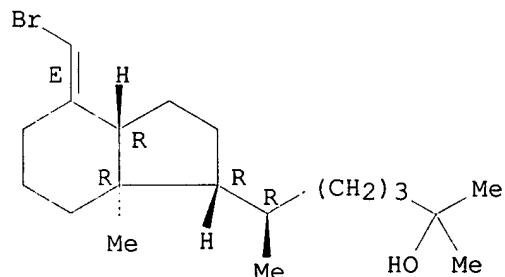
Absolute stereochemistry. Rotation (+).



RN 143705-63-9 HCAPLUS

CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



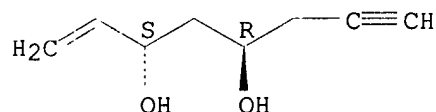
IT 152032-72-9P 161055-41-0P 169310-79-6P
169315-01-9P 203126-72-1P 203126-74-3P
203126-76-5P 203126-78-7P 203126-79-8P
203126-80-1P 203126-81-2P 203126-83-4P
203126-84-5P 203126-85-6P 203126-86-7P
203126-87-8P 203126-88-9P 203126-89-0P
203126-90-3P 203126-97-0P 203126-98-1P
203126-99-2P 203127-00-8P 203127-01-9P
203127-02-0P 203127-03-1P 203127-04-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3
analogs)

RN 152032-72-9 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

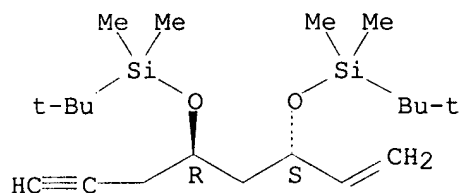
Absolute stereochemistry. Rotation (-).



RN 161055-41-0 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane,
5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-
propynyl)-, (5S,7R)- (9CI) (CA INDEX NAME)

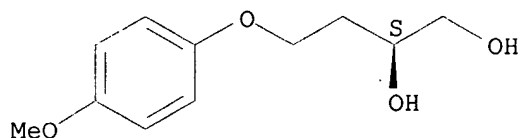
Absolute stereochemistry. Rotation (-).



RN 169310-79-6 HCAPLUS

CN 1,2-Butanediol, 4-(4-methoxyphenoxy)-, (S)- (9CI) (CA INDEX NAME)

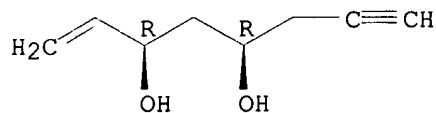
Absolute stereochemistry. Rotation (-).



RN 169315-01-9 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

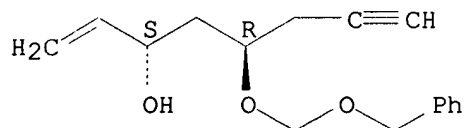
Absolute stereochemistry. Rotation (-).



RN 203126-72-1 HCAPLUS

CN 1-Octen-7-yn-3-ol, 5-[(phenylmethoxy)methoxy]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

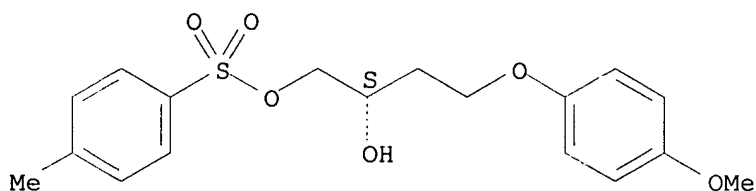
Absolute stereochemistry. Rotation (-).



RN 203126-74-3 HCAPLUS

CN 1,2-Butanediol, 4-(4-methoxyphenoxy)-, 1-(4-methylbenzenesulfonate), (S)- (9CI) (CA INDEX NAME)

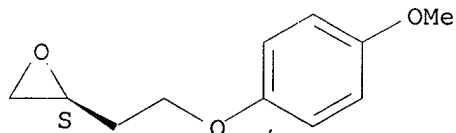
Absolute stereochemistry. Rotation (+).



RN 203126-76-5 HCAPLUS

CN Oxirane, [2-(4-methoxyphenoxy)ethyl]-, (S)- (9CI) (CA INDEX NAME)

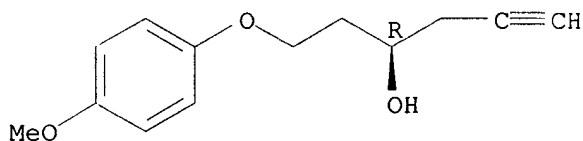
Absolute stereochemistry. Rotation (-).



RN 203126-78-7 HCAPLUS

CN 5-Hexyn-3-ol, 1-(4-methoxyphenoxy)-, (R)- (9CI) (CA INDEX NAME)

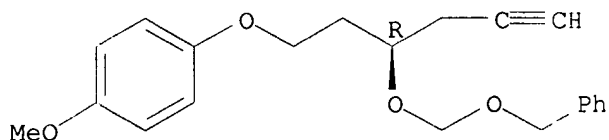
Absolute stereochemistry. Rotation (-).



RN 203126-79-8 HCAPLUS

CN Benzene, 1-methoxy-4-[[3-[(phenylmethoxy)methoxy]-5-hexynyl]oxy]-, (R)- (9CI) (CA INDEX NAME)

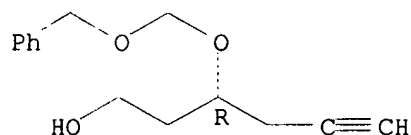
Absolute stereochemistry. Rotation (-).



RN 203126-80-1 HCAPLUS

CN 5-Hexyn-1-ol, 3-[(phenylmethoxy)methoxy]-, (R)- (9CI) (CA INDEX NAME)

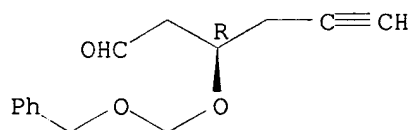
Absolute stereochemistry. Rotation (-).



RN 203126-81-2 HCAPLUS

CN 5-Hexynal, 3-[(phenylmethoxy)methoxy]-, (R)- (9CI) (CA INDEX NAME)

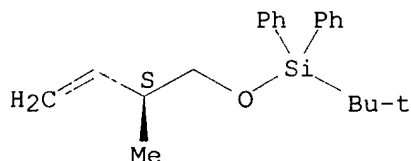
Absolute stereochemistry.



RN 203126-83-4 HCAPLUS

CN Silane, (1,1-dimethylethyl)[(2-methyl-3-butenyl)oxy]diphenyl-, (S)- (9CI)
(CA INDEX NAME)

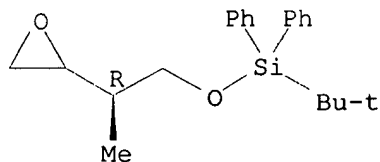
Absolute stereochemistry. Rotation (-).



RN 203126-84-5 HCAPLUS

CN Silane, (1,1-dimethylethyl)(2-oxiranylpropoxy)diphenyl-, [2(R)]- (9CI)
(CA INDEX NAME)

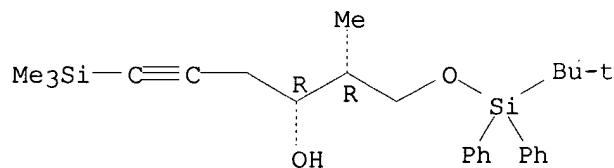
Absolute stereochemistry.



RN 203126-85-6 HCAPLUS

CN 5-Hexyn-3-ol, 1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

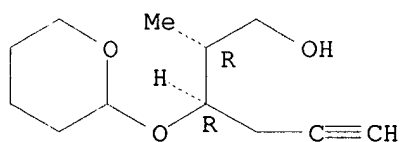
Absolute stereochemistry. Rotation (+).



RN 203126-86-7 HCAPLUS

CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-,
[2(2R,3R)]-[partial]- (9CI) (CA INDEX NAME)

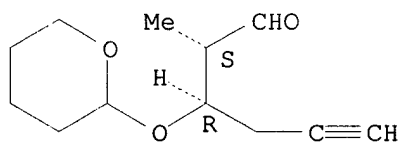
Absolute stereochemistry.



RN 203126-87-8 HCAPLUS

CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-,
[2(2S,3R)]-[partial]- (9CI) (CA INDEX NAME)

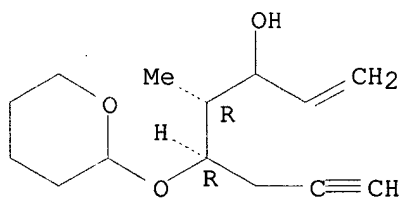
Absolute stereochemistry.



RN 203126-88-9 HCAPLUS

CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-,
[2(4R,5R)]-[partial]- (9CI) (CA INDEX NAME)

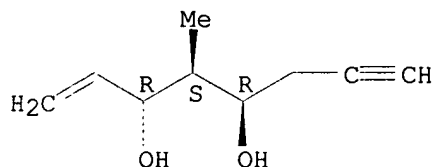
Absolute stereochemistry.



RN 203126-89-0 HCAPLUS

CN 1-Octen-7-yn-3,5-diol, 4-methyl-, [3R-(3R*,4S*,5R*)]- (9CI) (CA INDEX NAME)

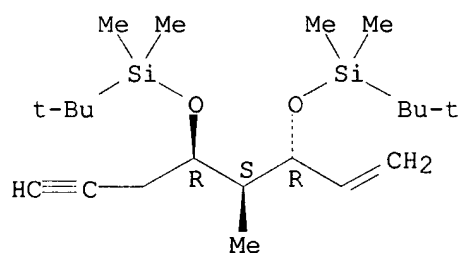
Absolute stereochemistry.



RN 203126-90-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

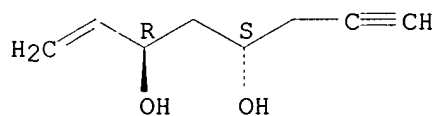
Absolute stereochemistry. Rotation (+).



RN 203126-97-0 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

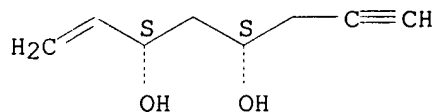
Absolute stereochemistry.



RN 203126-98-1 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

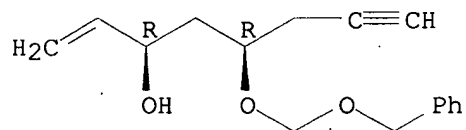
Absolute stereochemistry.



RN 203126-99-2 HCAPLUS

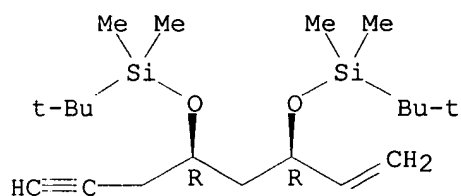
CN 1-Octen-7-yn-3-ol, 5-[(phenylmethoxy)methoxy]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



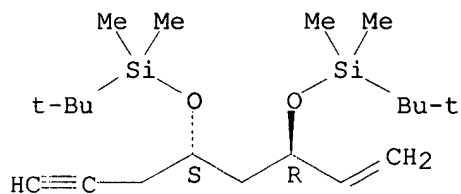
RN 203127-00-8 HCAPLUS
 CN 4,8-Dioxa-3,9-disilaundecane,
 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-
 propynyl)-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



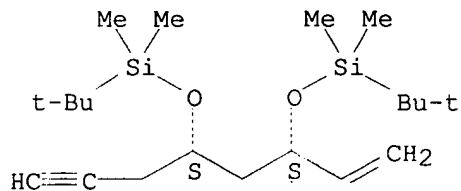
RN 203127-01-9 HCAPLUS
 CN 4,8-Dioxa-3,9-disilaundecane,
 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-
 propynyl)-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



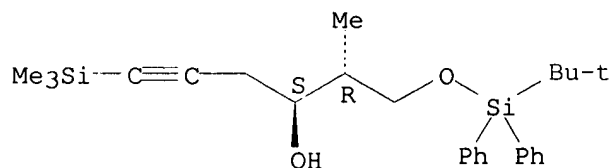
RN 203127-02-0 HCAPLUS
 CN 4,8-Dioxa-3,9-disilaundecane,
 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-
 propynyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 203127-03-1 HCAPLUS
 CN 5-Hexyn-3-ol, 1-[[[1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-
 (trimethylsilyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

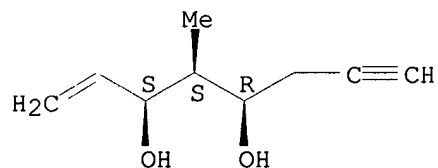
Absolute stereochemistry. Rotation (-).



RN 203127-04-2 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, 4-methyl-, [3S-(3R*,4R*,5S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 61476-45-7P 66791-71-7P 96614-28-7P

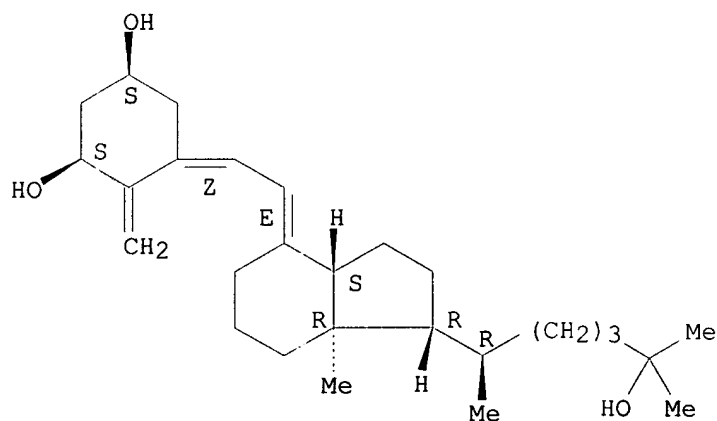
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)

RN 61476-45-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol,
(1.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

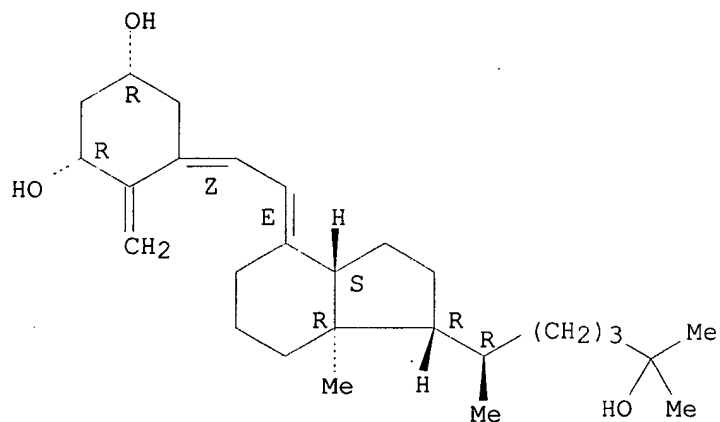


RN 66791-71-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol,
(1.beta.,3.beta.,5Z,7E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

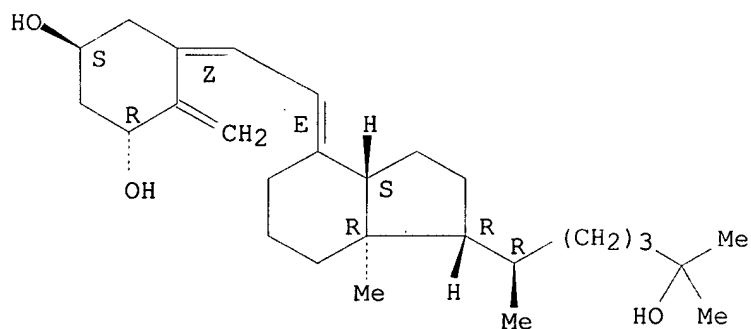


RN 96614-28-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol,
(1.β.,3.α.,5Z,7E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

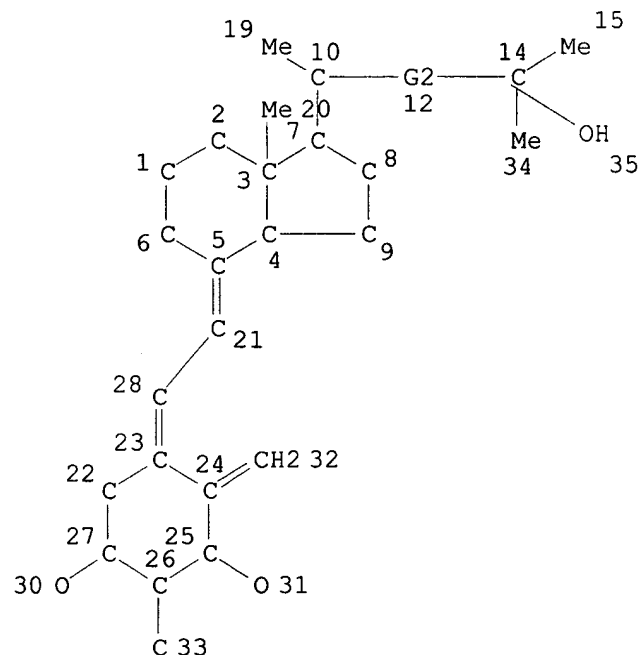
Double bond geometry as shown.



=> d que 122

L20

STR



REP G2=(2-4) CH2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L21 42 SEA FILE=BEILSTEIN SSS FUL L20

L22 42 SEA FILE=BEILSTEIN ABB=ON PLU=ON L21 AND PRE/FA

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L22 ANSWER 1 OF 42 BEILSTEIN COPYRIGHT 1999 BEILSTEIN CD&S

Beilstein Reg. No. (BRN): 8046533 Beilstein

Molecular Formula (MF): C40 H74 O3 Si2

Autonom Name (AUN):

6-(4-(2-<3,5-bis-(tert-butyl-dimethyl-silanyloxy)-4-

methyl-2-methylene-cyclohexylidene>-ethylidene)-7a-

methyl-octahydro-inden-1-yl)-2-methyl-heptan-2-ol

Beilstein Reference (SO): 6-06

General Comments (NTE): Stereo compound

Rltd. Stereoisomers (RSI): 7912362; 7912363; 7912364; 7912365; 7912366;
7912367; 7912368; 7912369; 8046526; 8046527;
8046528; 8046529; 8046530; 8046531; 8046532

Formula Weight (FW): 659.19

Lawson Number (LN): 6523; 3798; 3777

Ring System Data:

Number of Rings (CNR): 3

Ring Systems (CNRS): 2

Diff. Ring Systems (CNDRS): 2

Ring Heteros (CNRH): 0

Acyclic Heteros (CNAH): 5

Beilstein Ring Index (BRIX)	Ring System Formula (RF)	BRIX Count
9.2.5-0.0-0.0	C9	1
6.1.0-0.0-0.0	C6	1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Atom/Bond Notes:

1. CIP Descriptor: R
2. CIP Descriptor: S
3. CIP Descriptor: E
4. CIP Descriptor: Z

Preparation:

PRE

Start: BRN=7994164

6-(4-bromomethylene-7a-methyl-octahydro-inden-1-yl)-2-

methyl-heptan-2-ol, BRN=7907279 3,5-bis-(tert-butyl-dimethyl-
silanyloxy)-4-methyl-oct-1-en-7-yne

Reag: Pd2(dba)3, Ph3P, Et3N

Solv: CHCl3, toluene

Heating

Reference(s):

1. Fujishima, Toshie; Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu;
Ishizuka, Seiichi; et al., Bioorg.Med.Chem.Lett., 8 <1998> 16,
2145-2148, LA: EN, CODEN: BMCLE8

=> d

L24 ANSWER 1 OF 26 BEILSTEIN COPYRIGHT 1999 BEILSTEIN CD&S

Beilstein Reg. No. (BRN): 7912369 Beilstein

Molecular Formula (MF): C40 H74 O3 Si2

Autonom Name (AUN):

6-(4-(2-<3,5-bis-(tert-butyl-dimethyl-silanyloxy)-4-

methyl-2-methylene-cyclohexylidene>-ethylidene)-7a-

methyl-octahydro-inden-1-yl)-2-methyl-heptan-2-ol

Beilstein Reference (SO): 6-06

General Comments (NTE): Stereo compound

Rltd. Stereoisomers (RSI): 7912362; 7912363; 7912364; 7912365; 7912366;
7912367; 7912368; 8046526; 8046527; 8046528;
8046529; 8046530; 8046531; 8046532; 8046533

Formula Weight (FW): 659.19

Lawson Number (LN): 6523; 3798; 3777

Ring System Data:

Number of Rings (CNR): 3

Ring Systems (CNRS): 2

Diff. Ring Systems (CNDRS): 2

Ring Heteros (CNRH): 0

Acyclic Heteros (CNAH): 5

Beilstein Ring Index (BRIX)	Ring System Formula (RF)	BRIX Count
9.2.5-0.0-0.0	C9	1
6.1.0-0.0-0.0	C6	1

Preparation:

PRE

Start: BRN=7907279

3,5-bis-(tert-butyl-dimethyl-silanyloxy)-4-methyl-oct-

1-en-7-yne, BRN=5868945 6-(4-bromomethylene-7a-methyl-octahydro-
inden-1-yl)-2-methyl-heptan-2-ol

Reag: Pd2(dba)3PPh3, Et3N

Solv: toluene

Temp: 120.0 Cel

Reference(s):

1. Konno, Katsuhiro; Maki, Shojiro; Fujishima, Toshie; Liu, Zhaopeng;
Miura, Daishiro; et al., Bioorg.Med.Chem.Lett., 8 <1998> 2, 151-156,
LA: EN, CODEN: BMCLE8

=> d

L27 ANSWER 1 OF 10 BEILSTEIN COPYRIGHT 1999 BEILSTEIN CD&S

Beilstein Reg. No. (BRN): 7837289 Beilstein
Molecular Formula (MF): C33 H56 O4
Autonom Name (AUN): 5-(2-<1-(5-hydroxy-1,5-dimethyl-hexyl)-7a-methyl-

octahydro-inden-4-ylidene>-ethylidene)-2-(6-hydroxy-
hexyl)-4-methylene-cyclohexane-1,3-diol

Beilstein Reference (SO): 6-06
General Comments (NTE): Stereo compound
Formula Weight (FW): 516.80
Lawson Number (LN): 6704

Ring System Data:

Number of Rings (CNR): 3
Ring Systems (CNRS): 2
Diff. Ring Systems (CNDRS): 2
Ring Heteros (CNRH): 0
Acyclic Heteros (CNAH): 4

Beilstein Ring Index (BRIX)	Ring System Formula (RF)	BRIX Count
9.2.5-0.0-0.0	C9	1
6.1.0-0.0-0.0	C6	1

Preparation:

PRE

Start: BRN=7836562 (2R)-2-(6-hydroxyhexyl)-1.alpha.,3.beta.,25-
trihydroxycholesta-5,7-diene

Detail: 1.) EtOH, 0 deg C, 2 min, irradi. 2.) EtOH, 2 h, reflux

Reference(s):

1. Ono, Yoshiyuki; Watanabe, Hiroyoshi; Shiraishi, Ayako; Takeda,
Satoshi;

Higuchi, Yoshinobu; et al., Chem.Pharm.Bull., 45 <1997> 10, 1626-1630,
LA: EN, CODEN: CPBTAL

Note(s):

2. Yield given. Multistep reaction

=> d

L30 ANSWER 1 OF 5 BEILSTEIN COPYRIGHT 1999 BEILSTEIN CD&S

Beilstein Reg. No. (BRN): 7343182 Beilstein
 Molecular Formula (MF): C31 H51 F O3
 Autonom Name (AUN):
 2-(4-fluoro-butyl)-5-(2-<1-(5-hydroxy-1,5-dimethyl-
 hexyl)-7a-methyl-octahydro-inden-4-ylidene>-
 ethylidene)-4-methylene-cyclohexane-1,3-diol
 Beilstein Reference (SO): 6-06
 General Comments (NTE): Stereo compound
 Rltd. Stereoisomers (RSI): 7343181
 Formula Weight (FW): 490.74
 Lawson Number (LN): 6526

Ring System Data:

Number of Rings (CNR): 3
 Ring Systems (CNRS): 2
 Diff. Ring Systems (CNDRS): 2
 Ring Heteros (CNRH): 0
 Acyclic Heteros (CNAH): 4

Beilstein Ring Index (BRIX)	Ring System Formula (RF)	BRIX Count
9.2.5-0.0-0.0	C9	1
6.1.0-0.0-0.0	C6	1

Preparation:

PRE

Start: BRN=7326668 4-(2-<3,5-bis-(tert-butyl-dimethyl-silanyloxy)-4-(4-
 fluoro-butyl)-2-methylene-cyclohexylidene>-ethylidene)-1-<5-(tert-
 butyl-dimethyl-silanyloxy)-1,5-dimethyl-hexyl>-7a-methyl-octahydro-
 indene

Reag: n-Bu4NF, 4 Angstroem molecular sieves
 Time: 3.5 hour(s)
 Solv: tetrahydrofuran
 Temp: 60.0 Cel

ByProd: BRN=7343181 2-(4-fluoro-butyl)-5-(2-<1-(5-hydroxy-1,5-dimethyl-
 hexyl)-7a-methyl-octahydro-inden-4-ylidene>-ethylidene)-4-
 methylene-cyclohexane-1,3-diol

Reference(s):

1. Posner, Gary H.; Cho, Cheon-Gyu; Anjeh, Tizah E. N.; Johnson, Neil;
 Horst, Ronald L.; et al., J.Org.Chem., 60 <1995> 14, 4617-4628, LA:

EN,

CODEN: JOCEAH

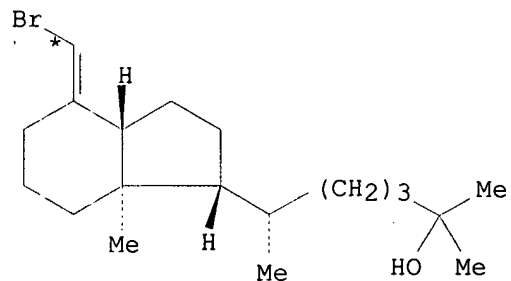
Note(s):

2. Yield given. Yields of byproduct given

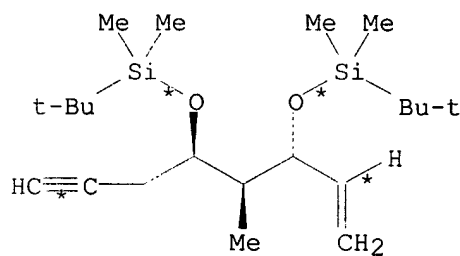
=> d fhit bib abs

L38 ANSWER 1 OF 1 CASREACT COPYRIGHT 1999 ACS

RX(1) OF 1 A + B ==> C

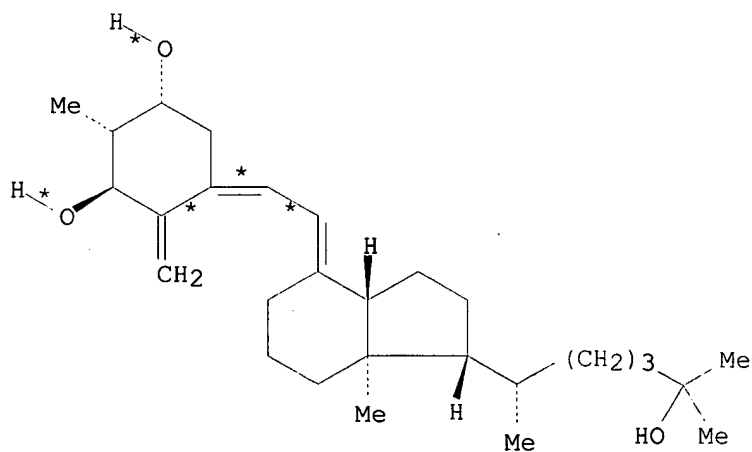


A



B

(1) →



C

RX(1) RCT A 214351-89-0, B 203126-90-3
 RGT D 121-44-8 Et3N, E 603-35-0 PPh3
 PRO C 214351-93-6
 CAT 52522-40-4 Pd complex
 SOL 108-88-3 PhMe

AN 129:343629 CASREACT

TI Preparation of vitamin D3 derivatives and their pharmaceutical uses

IN Takayama, Hiroaki; Konno, Katsuhiro; Fujishima, Toshie
 PA Teijin Ltd., Japan
 SO PCT Int. Appl., 57 pp.
 CODEN: PIXXD2
 DT Patent
 LA Japanese
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9850353	A1	19981112	WO 98-JP1979	19980430
	W: JP, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI	JP 97-114695		19970502		
OS	MARPAT 129:343629				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 1,25-Dihydroxy-2-Me vitamin D3 derivs. I [R1, R2 = H, tri(C1-7alkyl)silyl; the asym. carbon atoms at the 1-, 2- and 3-positions each independently has an .alpha.- or .beta.-configuration], useful as remedies for osteoporosis, rachitis, accessory thyroidal hyperenergia, etc., are prepd. via reaction of II (X = bromo, iodo) with III (R3, R4 = H, trihydrocarbylsilyl) in the presence of a palladium catalyst optionally followed by deprotection (removal of silyl groups). Thus, II (X = Br) was reacted with III (R3 = R4 = TBS) in toluene contg. Et3N, Pd2(dba)3.CHCl3, and Ph3P at 120.degree. to give IV (R = TBS), which was treated with camphor-10-sulfonic acid in methanol to give 63% IV (R = H). In a study using 1.alpha.,25-dihydroxyvitamin D3 receptors in the bovine thymus gland, this showed an affinity of 160 compared with 100 for 1.alpha.,25-dihydroxyvitamin D3.

=> D HIS

(FILE 'HOME' ENTERED AT 14:02:27 ON 22 JUN 1999)

FILE 'HCAPLUS' ENTERED AT 14:02:33 ON 22 JUN 1999

L1 719 S TAKAYAMA H?/AU
L2 896 S KONNO K?/AU
L3 172 S FUJISHIMA T?/AU
L4 4 S L1 AND L2 AND L3
SELECT RN L4 1-4

FILE 'HCAPLUS' ENTERED AT 14:03:07 ON 22 JUN 1999

FILE 'REGISTRY' ENTERED AT 14:03:23 ON 22 JUN 1999

L5 96 S E1-96

FILE 'HCAPLUS' ENTERED AT 14:03:41 ON 22 JUN 1999

L6 3 S L4 AND L5
L7 1 S L4 NOT L6

=> D ALL

L7 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:710271 HCAPLUS
TI Corrigendum to "A novel and practical route to A-ring enyne synthon for
1.alpha.,25-dihydroxyvitamin D3 analogs: synthesis of A-ring
diastereomers
of 1.alpha.,25-dihydroxy-vitamin D3 and 2-methyl-1,25-dihydroxyvitamin
D3"
AU Konno, Katsuhiko; Maki, Shojiro; Fujishima, Toshie;
Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu; Takayama, Hiroaki
CS Faculty of Pharmaceutical Sciences, Teikyo University, Sagamiko,
Kanagawa,
199-01, Japan
SO Bioorg. Med. Chem. Lett. (1998), 8(19), 2817
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal; Errata
LA English
AB Unavailable

=> D L6 BIB ABS HITSTR

L6 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 1999 ACS
 AN 1998:745027 HCAPLUS
 DN 129:343629
 TI Preparation of vitamin D3 derivatives and their pharmaceutical uses
 IN Takayama, Hiroaki; Konno, Katsuhiko; Fujishima, Toshie
 PA Teijin Ltd., Japan
 SO PCT Int. Appl., 57 pp.
 CODEN: PIXXD2
 DT Patent
 LA Japanese
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9850353	A1	19981112	WO 98-JP1979	19980430
	W: JP, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI	JP 97-114695		19970502		
OS	CASREACT 129:343629; MARPAT 129:343629				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

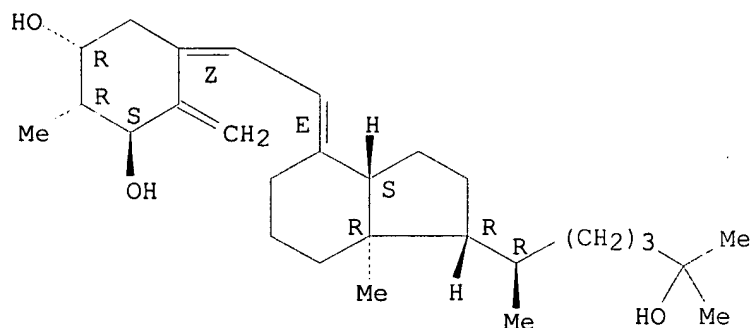
AB 1,25-Dihydroxy-2-Me vitamin D3 derivs. I [R1, R2 = H, tri(C1-7alkyl)silyl; the asym. carbon atoms at the 1-, 2- and 3-positions each independently has an .alpha.- or .beta.-configuration], useful as remedies for osteoporosis, rachitis, accessory thyroidal hyperenergia, etc., are prepd. via reaction of II (X = bromo, iodo) with III (R3, R4 = H, trihydrocarbylsilyl) in the presence of a palladium catalyst optionally followed by deprotection (removal of silyl groups). Thus, II (X = Br) was reacted with III (R3 = R4 = TBS) in toluene contg. Et3N, Pd2(dba)3.CHCl3, and Ph3P at 120.degree. to give IV (R = TBS), which was treated with camphor-10-sulfonic acid in methanol to give 63% IV (R = H). In a study using 1.alpha.,25-dihydroxyvitamin D3 receptors in the bovine thymus gland, this showed an affinity of 160 compared with 100 for 1.alpha.,25-dihydroxyvitamin D3.

IT 158388-11-5P 214351-93-6P 214351-94-7P
 214351-95-8P 214351-96-9P 214351-97-0P
 214351-98-1P 214351-99-2P 215394-65-3P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of vitamin D3 derivs. and their pharmaceutical uses)

RN 158388-11-5 HCAPLUS
 CN 9,10-Seccholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-, (1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

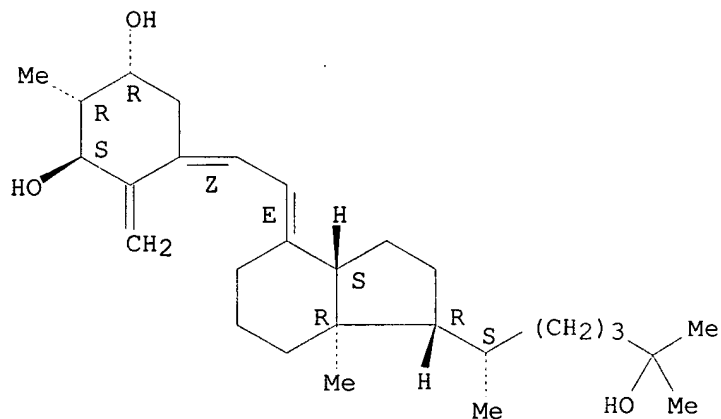


RN 214351-93-6 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

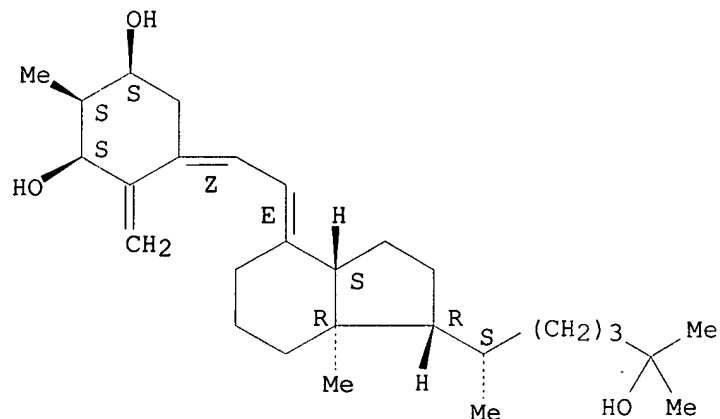


RN 214351-94-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

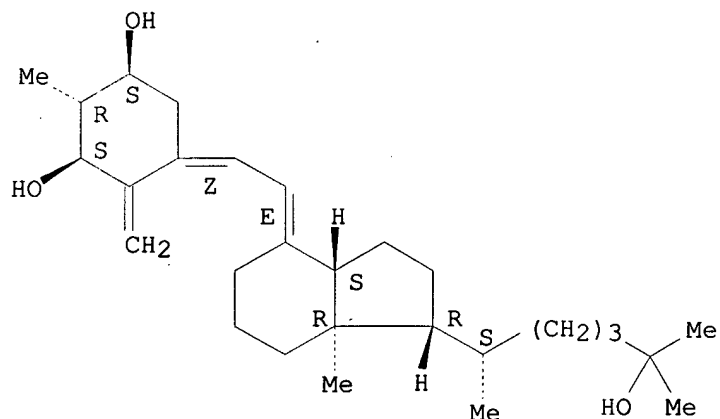


RN 214351-95-8 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

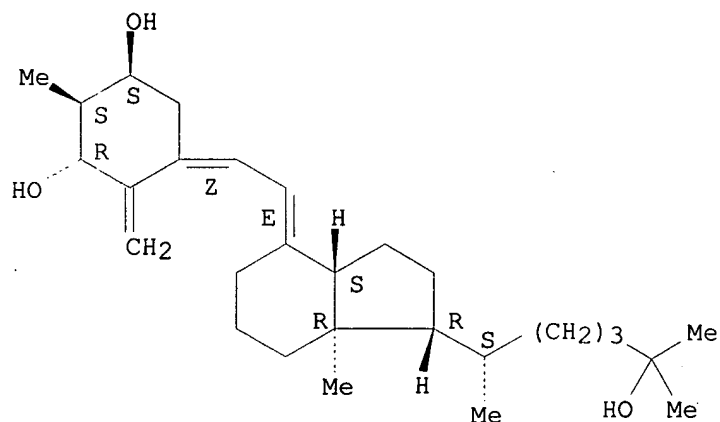


RN 214351-96-9 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.beta.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

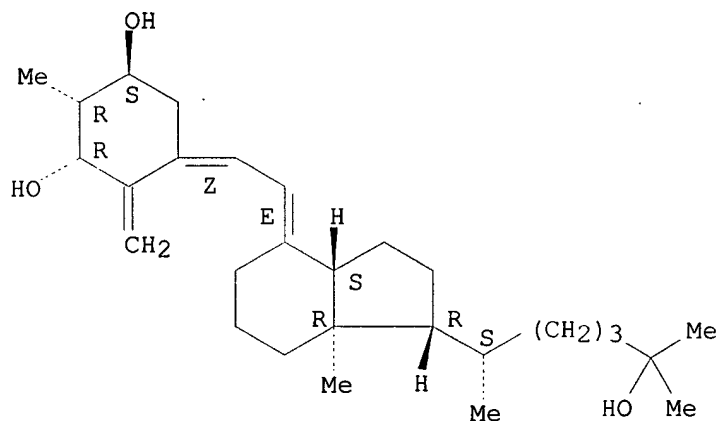


RN 214351-97-0 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.α.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

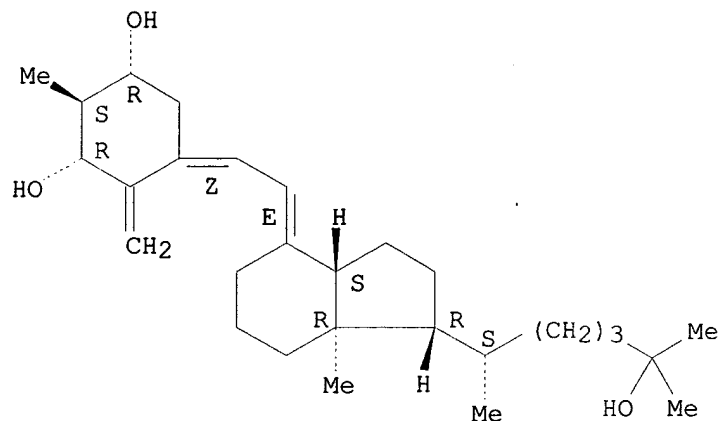


RN 214351-98-1 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.α.,3.β.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

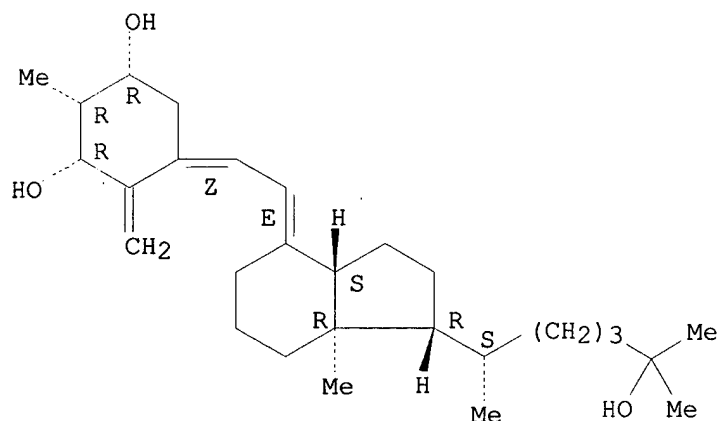


RN 214351-99-2 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.β.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

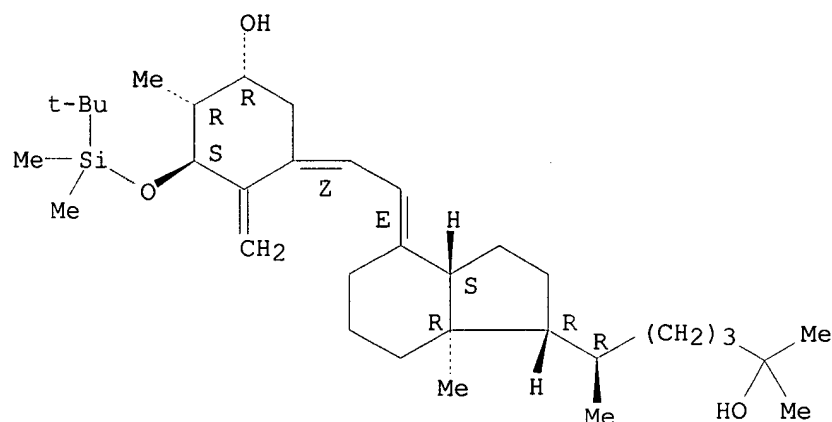


RN 215394-65-3 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-3,25-triol, 1-[[[(1,1-
dimethylethyl)dimethylsilyl]oxy]-2-methyl-,
(1.α.,2.β.,3.β.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 52522-40-4

RL: CAT (Catalyst use); USES (Uses)

(prepn. of vitamin D3 derivs. and their pharmaceutical uses)

RN 52522-40-4 HCAPLUS

CN Palladium, tris[.mu.-[(1,2-.eta.:4,5-.eta.)-(1E,4E)-1,5-diphenyl-1,4-pentadien-3-one]]di-, compd. with trichloromethane (1:1) (9CI) (CA INDEX NAME)

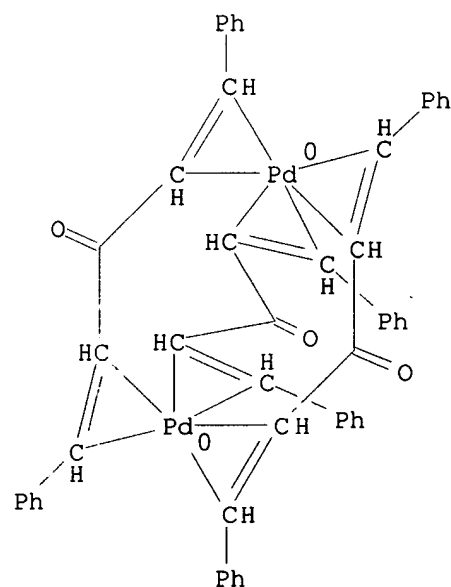
CM 1

CRN 51364-51-3

CMF C51 H42 O3 Pd2

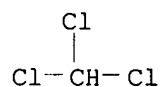
CCI CCS

CDES 2:ALL,E

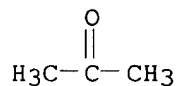


CM 2

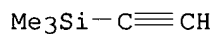
CRN 67-66-3
CMF C H Cl3



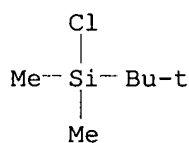
IT 67-64-1, 2-Propanone, reactions 1066-54-2,
Ethynyltrimethylsilane 18162-48-6, tert-Butyldimethylsilyl
chloride 20445-33-4 39637-99-5 69739-34-0,
tert-Butyldimethylsilyl triflate 143705-63-9 214351-89-0
RL: RCT (Reactant)
(prepn. of vitamin D3 derivs. and their pharmaceutical uses)
RN 67-64-1 HCAPLUS
CN 2-Propanone (9CI) (CA INDEX NAME)



RN 1066-54-2 HCAPLUS
CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

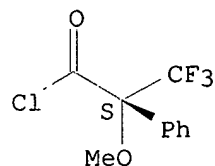


RN 18162-48-6 HCAPLUS
CN Silane, chloro(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



RN 20445-33-4 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-,
(.alpha.S)- (9CI) (CA INDEX NAME)

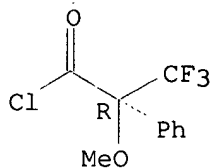
Absolute stereochemistry. Rotation (+).



RN 39637-99-5 HCAPLUS
CN Benzeneacetyl chloride, .alpha.-methoxy-.alpha.-(trifluoromethyl)-,

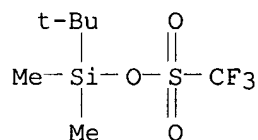
(.alpha.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 69739-34-0 HCAPLUS

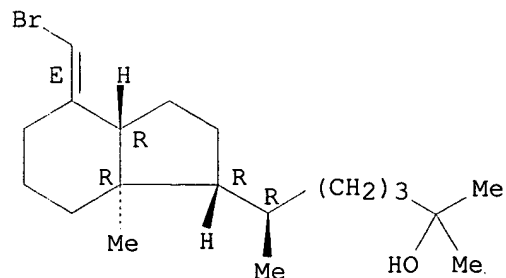
CN Methanesulfonic acid, trifluoro-, (1,1-dimethylethyl)dimethylsilyl ester
(9CI) (CA INDEX NAME)



RN 143705-63-9 HCAPLUS

CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-
.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)-
(9CI) (CA INDEX NAME)

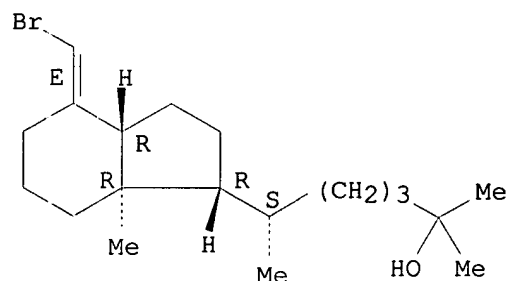
Absolute stereochemistry.
Double bond geometry as shown.



RN 214351-89-0 HCAPLUS

CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-
.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4E,7aR)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 104701-87-3P 112057-64-4P 147915-53-5P
 147915-54-6P 203126-90-3P 215394-09-5P
 215394-10-8P 215394-12-0P 215394-15-3P
 215394-17-5P 215394-20-0P 215394-22-2P
 215394-23-3P 215394-24-4P 215394-25-5P
 215394-26-6P 215394-27-7P 215394-28-8P
 215394-29-9P 215394-30-2P 215394-31-3P
 215394-32-4P 215394-33-5P 215394-34-6P
 215394-35-7P 215394-36-8P 215394-37-9P
 215394-38-0P

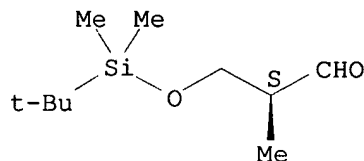
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of vitamin D₃ derivs. and their pharmaceutical uses)

RN 104701-87-3 HCAPLUS

CN Propanal, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (2S)-
 (9CI)

(CA INDEX NAME)

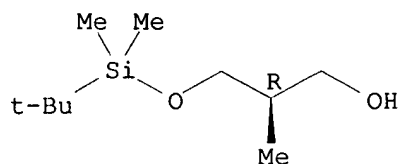
Absolute stereochemistry.



RN 112057-64-4 HCAPLUS

CN 1-Propanol, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-, (2R)-
 (9CI) (CA INDEX NAME)

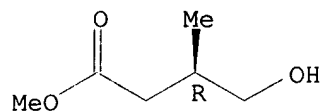
Absolute stereochemistry. Rotation (+).



RN 147915-53-5 HCAPLUS

CN Butanoic acid, 4-hydroxy-3-methyl-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

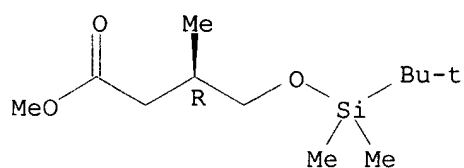
Absolute stereochemistry.



RN 147915-54-6 HCAPLUS

CN Butanoic acid, 4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-methyl-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

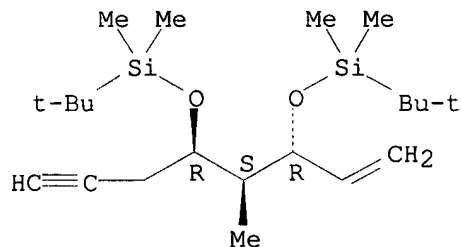
Absolute stereochemistry.



RN 203126-90-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

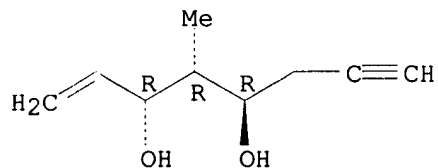
Absolute stereochemistry. Rotation (+).



RN 215394-09-5 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3R,4R,5R)- (9CI) (CA INDEX NAME)

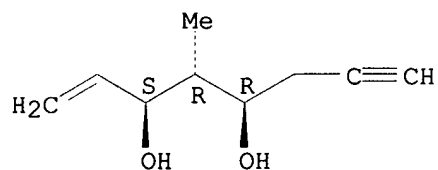
Absolute stereochemistry.



RN 215394-10-8 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, 4-methyl-, (3S,4R,5R)- (9CI) (CA INDEX NAME)

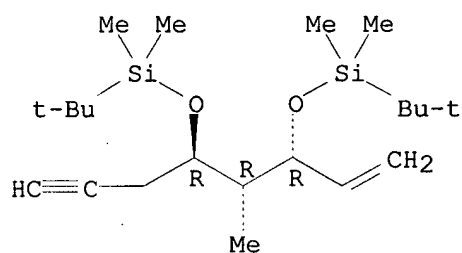
Absolute stereochemistry.



RN 215394-12-0 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7R)- (9CI) (CA INDEX NAME)

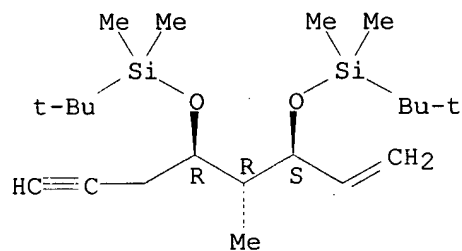
Absolute stereochemistry.



RN 215394-15-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7R)- (9CI) (CA INDEX NAME)

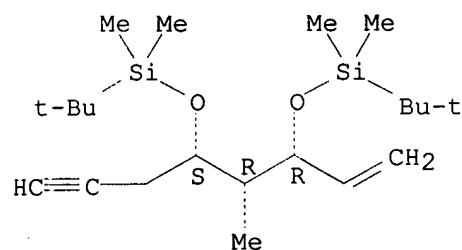
Absolute stereochemistry.



RN 215394-17-5 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6R,7S)- (9CI) (CA INDEX NAME)

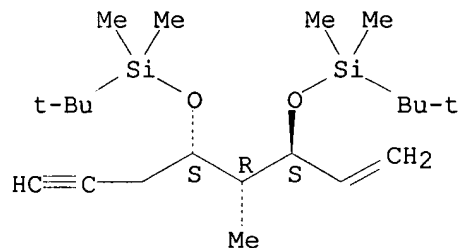
Absolute stereochemistry.



RN 215394-20-0 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6R,7S)- (9CI) (CA INDEX NAME)

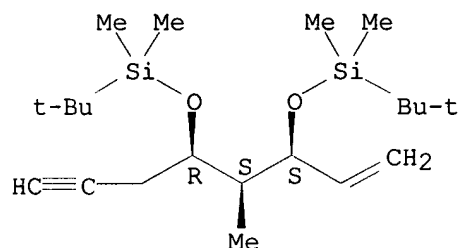
Absolute stereochemistry.



RN 215394-22-2 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7R)- (9CI) (CA INDEX NAME)

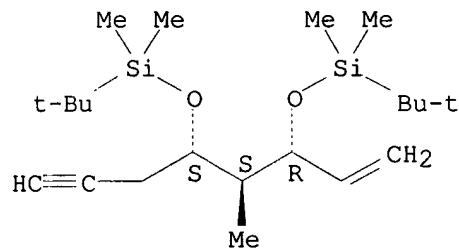
Absolute stereochemistry.



RN 215394-23-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7S)- (9CI) (CA INDEX NAME)

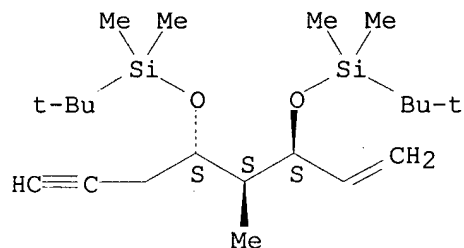
Absolute stereochemistry.



RN 215394-24-4 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5S,6S,7S)- (9CI) (CA INDEX NAME)

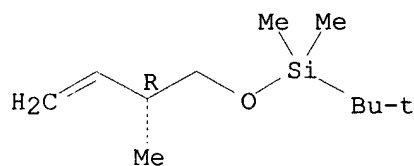
Absolute stereochemistry.



RN 215394-25-5 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[[(2R)-2-methyl-3-butenyl]oxy]- (9CI)
(CA INDEX NAME)

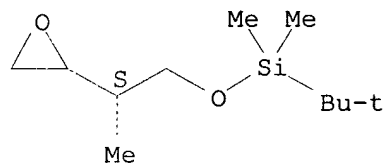
Absolute stereochemistry.



RN 215394-26-6 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[(2S)-2-oxiranylpropoxy]- (9CI) (CA
INDEX NAME)

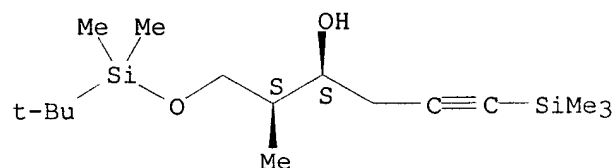
Absolute stereochemistry.



RN 215394-27-7 HCAPLUS

CN 5-Hexyn-3-ol, 1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3S)- (9CI) (CA INDEX NAME)

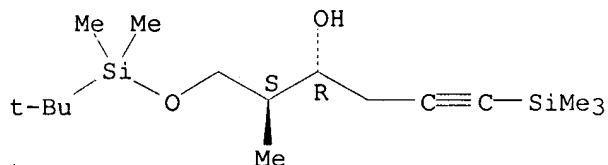
Absolute stereochemistry.



RN 215394-28-8 HCAPLUS

CN 5-Hexyn-3-ol, 1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, (2S,3R)- (9CI) (CA INDEX NAME)

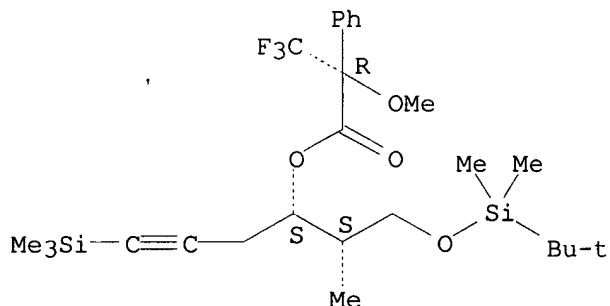
Absolute stereochemistry.



RN 215394-29-9 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1S)-1-[(1S)-2-[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

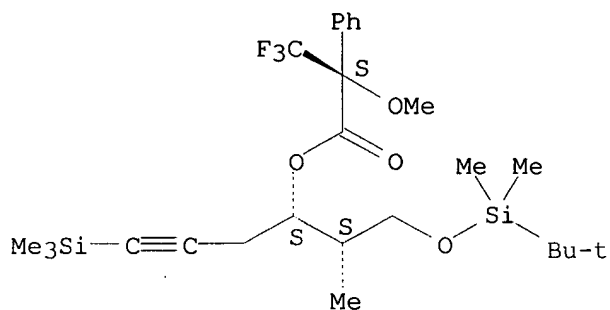
Absolute stereochemistry.



RN 215394-30-2 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

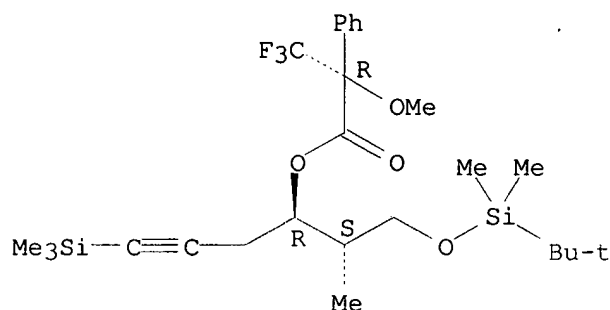
Absolute stereochemistry.



RN 215394-31-3 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.R)- (9CI) (CA INDEX NAME)

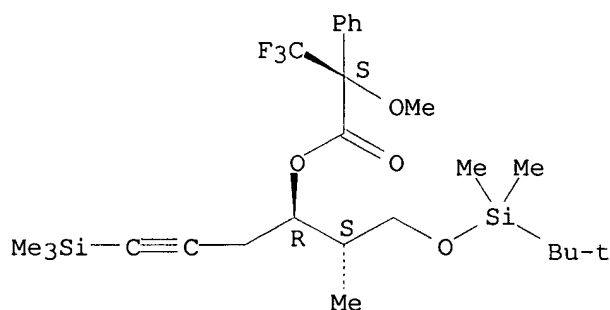
Absolute stereochemistry.



RN 215394-32-4 HCAPLUS

CN Benzeneacetic acid, .alpha.-methoxy-.alpha.-(trifluoromethyl)-, (1R)-1-[(1S)-2-[[1,1-dimethylethyl]dimethylsilyl]oxy]-1-methylethyl]-4-(trimethylsilyl)-3-butynyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

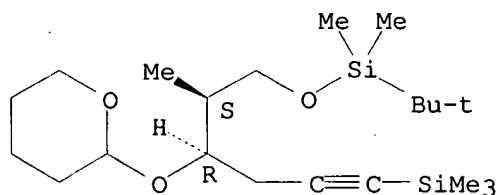
Absolute stereochemistry.



RN 215394-33-5 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[(2S,3R)-2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-3-[3-(trimethylsilyl)-2-propynyl]propoxy]- (9CI) (CA INDEX NAME)

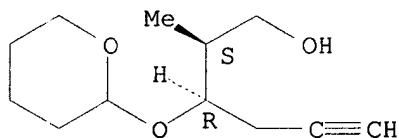
Absolute stereochemistry.



RN 215394-34-6 HCAPLUS

CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2S,3R)- (9CI) (CA INDEX NAME)

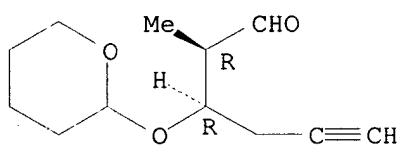
Absolute stereochemistry.



RN 215394-35-7 HCAPLUS

CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (2R,3R)- (9CI)
(CA INDEX NAME)

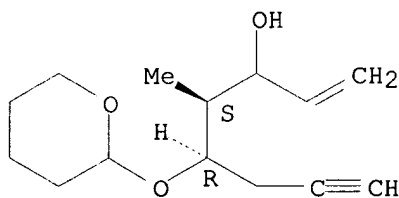
Absolute stereochemistry.



RN 215394-36-8 HCAPLUS

CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, (4S,5R)-
(9CI) (CA INDEX NAME)

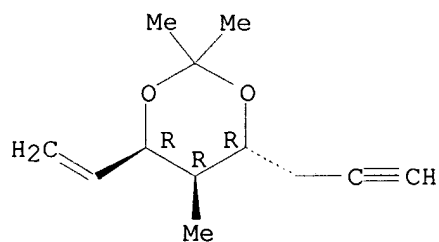
Absolute stereochemistry.



RN 215394-37-9 HCAPLUS

CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4R,5R,6R)- (9CI)
(CA INDEX NAME)

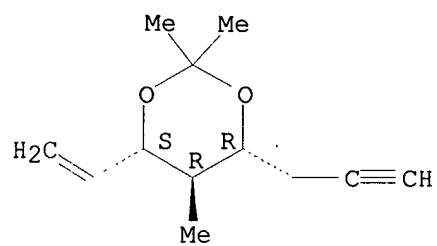
Absolute stereochemistry.



RN 215394-38-0 HCAPLUS

CN 1,3-Dioxane, 4-ethenyl-2,2,5-trimethyl-6-(2-propynyl)-, (4S,5R,6R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



=> D L6 BIB ABS HITSTR 2

L6 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 1999 ACS

AN 1998:606883 HCAPLUS

DN 129:290279

TI Synthesis and biological activity of 2-methyl-20-epi analogs of
1.alpha.,25-dihydroxyvitamin D3

AU **Fujishima, Toshie**; Liu, Zhaopeng; Miura, Daishiro; Chokki,
Manabu; Ishizuka, Seiichi; **Konno, Katsuhiko**; **Takayama,**
Hiroaki

CS Faculty of Pharmaceutical Sciences, Teikyo University, Kanagawa,
199-0195.

SO Bioorg. Med. Chem. Lett. (1998), 8(16), 2145-2148

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

AB Synthesis and biol. evaluation of all eight possible A-ring diastereomers of 2-methyl-20-epi-1,25-dihydroxyvitamin D3 are described. Among the analogs synthesized, 2.alpha.-methyl-20-epi-1.alpha.,25-dihydroxyvitamin D3 exhibited exceptionally high potency. The double modification of 2-Me substitution and 20-epimerization yielded analogs with unique activity profiles.

IT 32222-06-3P, 1.alpha.,25-Dihydroxyvitamin D3

RL: PNU (Preparation, unclassified); PREP (Preparation)

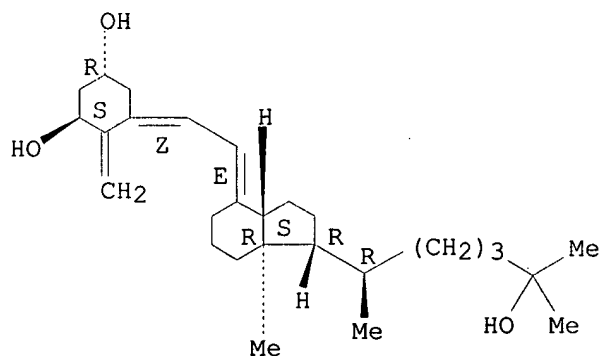
(Synthesis and biol. activity of 2-methyl-20-epi analogs of 1.alpha.,25-dihydroxyvitamin D3)

RN 32222-06-3 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol,
(1.alpha.,3.beta.,5Z,7E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 214351-84-5P 214351-93-6P 214351-94-7P

214351-95-8P 214351-96-9P 214351-97-0P

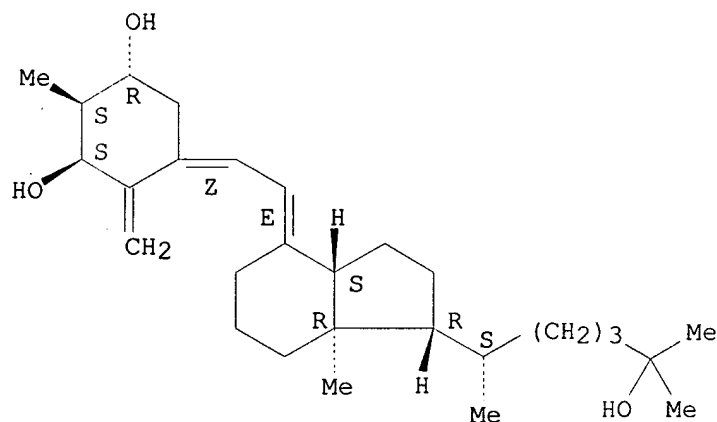
214351-98-1P 214351-99-2P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biol. activity of 2-methyl-20-epi analogs of

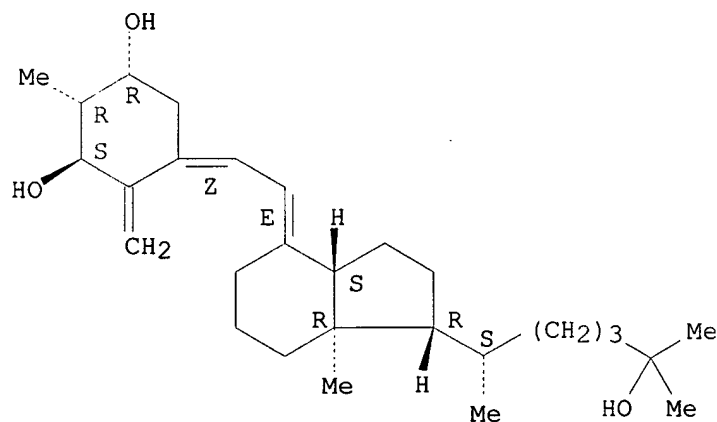
1.alpha.,25-dihydroxyvitamin D3)
RN 214351-84-5 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



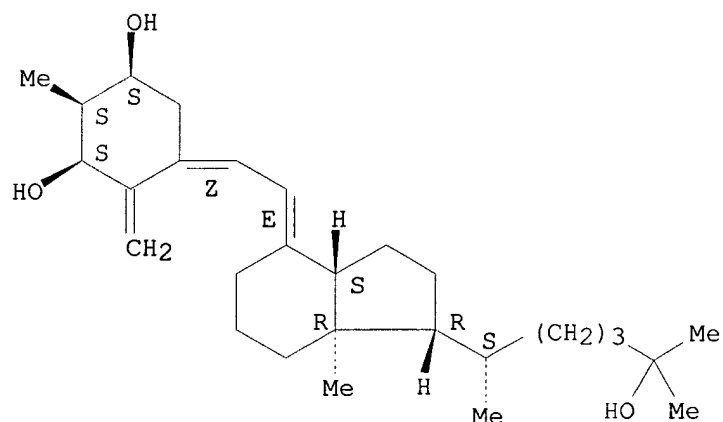
RN 214351-93-6 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.beta.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 214351-94-7 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

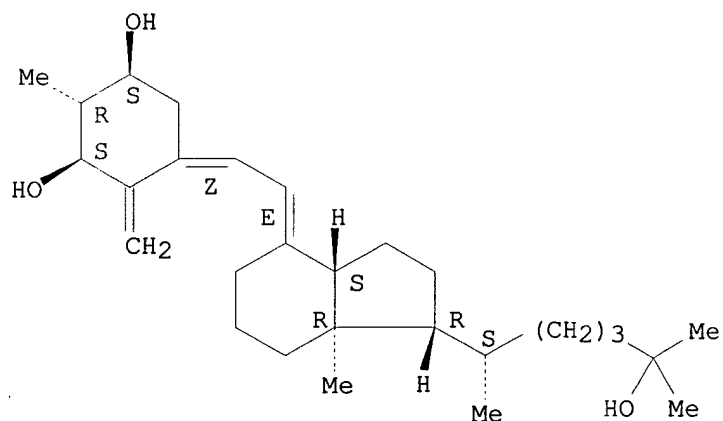


RN 214351-95-8 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

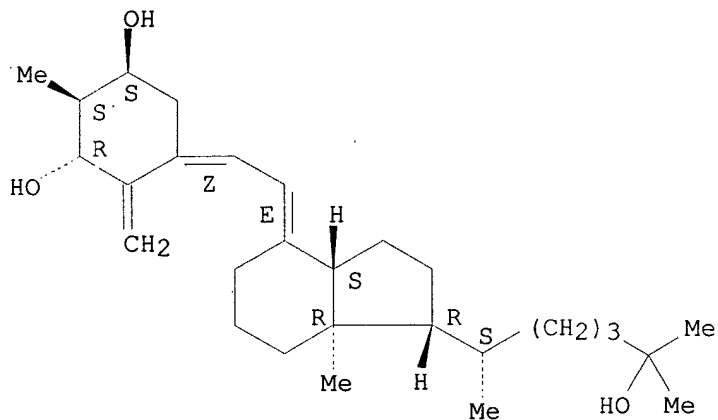


RN 214351-96-9 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.beta.,2.alpha.,3.alpha.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

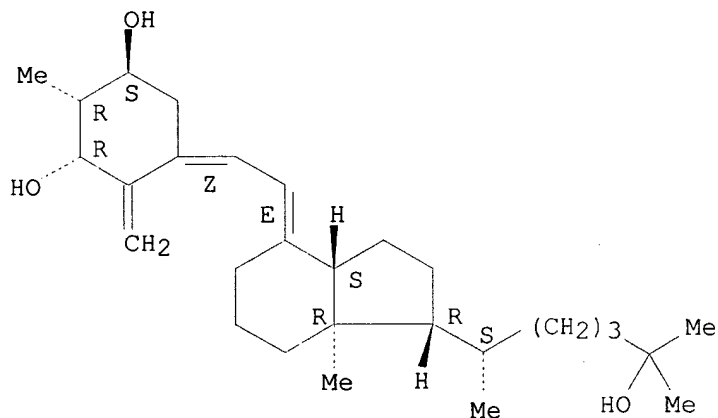
Double bond geometry as shown.



RN 214351-97-0 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.α.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

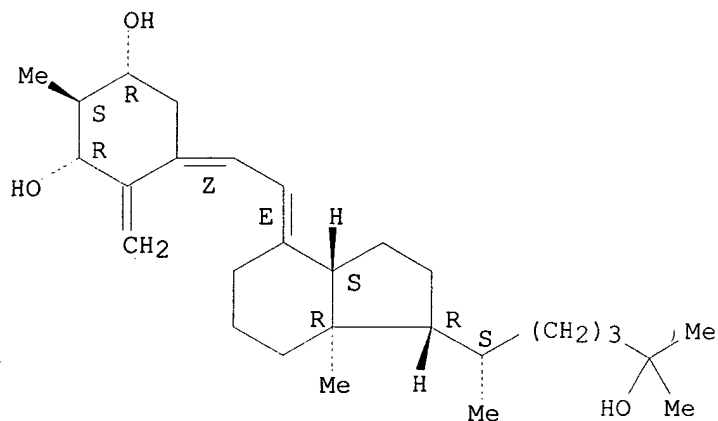
Absolute stereochemistry.
Double bond geometry as shown.



RN 214351-98-1 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.α.,3.β.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

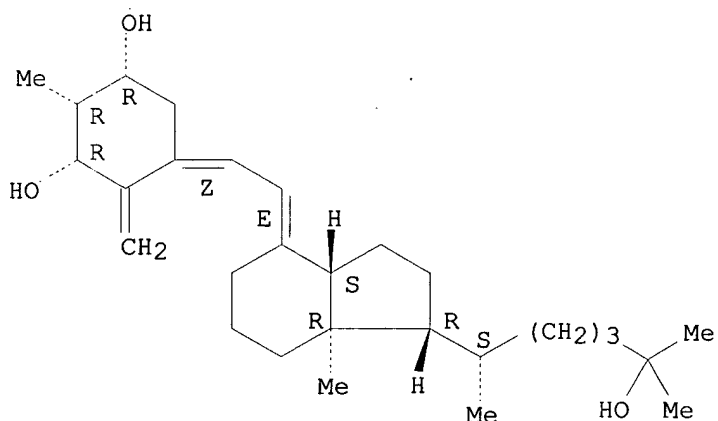


RN 214351-99-2 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.β.,5Z,7E,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 104651-47-0 203126-90-3 214351-87-8

RL: RCT (Reactant)

(synthesis and biol. activity of 2-methyl-20-epi analogs of
1.α.,25-dihydroxyvitamin D3)

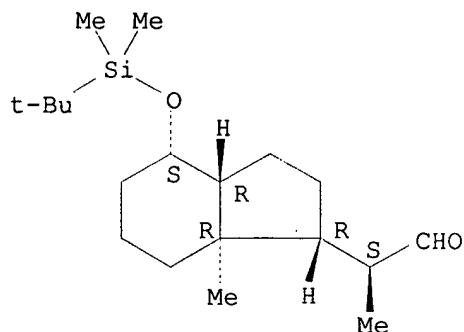
RN 104651-47-0 HCAPLUS

CN 1H-Indene-1-acetaldehyde,

4-[[[1,1-dimethylethyl)dimethylsilyl]oxy]octahyd

ro-α.,7a-dimethyl-, (.α.S,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

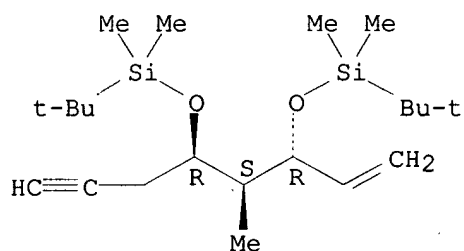
Absolute stereochemistry. Rotation (+).



RN 203126-90-3 HCAPLUS

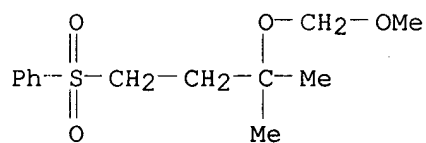
CN 4,8-Dioxo-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 214351-87-8 HCAPLUS

CN Benzene, [[3-(methoxymethoxy)-3-methylbutyl]sulfonyl]- (9CI) (CA INDEX NAME)



IT 171011-48-6P 183506-75-4P 213250-67-0P

214351-86-7P 214351-88-9P 214351-89-0P

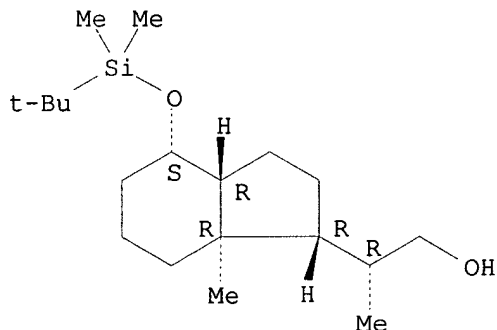
214351-91-4P 214351-92-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and biol. activity of 2-methyl-20-epi analogs of
1.alpha.,25-dihydroxyvitamin D3)

RN 171011-48-6 HCAPLUS

CN 1H-Indene-1-ethanol, 4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.beta.,7a-dimethyl-, (.beta.R,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

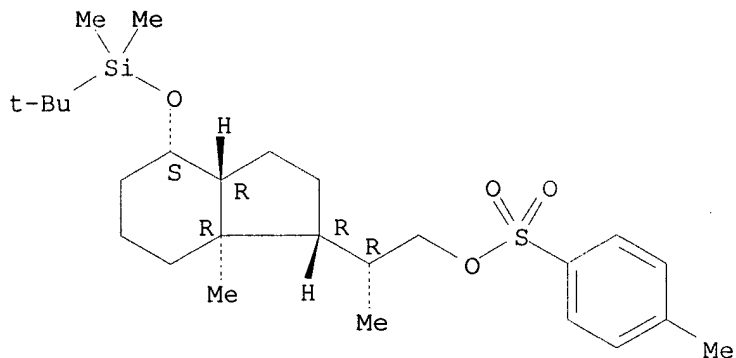
Absolute stereochemistry. Rotation (+).



RN 183506-75-4 HCAPLUS

CN 1H-Indene-1-ethanol, 4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]octahydro-.beta.,7a-dimethyl-, 4-methylbenzenesulfonate, (.beta.R,1R,3aR,4S,7aR)-(9CI) (CA INDEX NAME)

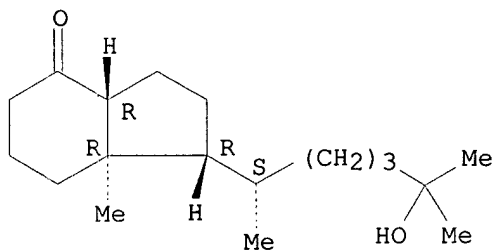
Absolute stereochemistry. Rotation (+).



RN 213250-67-0 HCAPLUS

CN 4H-Inden-4-one, octahydro-1-[(1S)-5-hydroxy-1,5-dimethylhexyl]-7a-methyl-, (1R,3aR,7aR)-(9CI) (CA INDEX NAME)

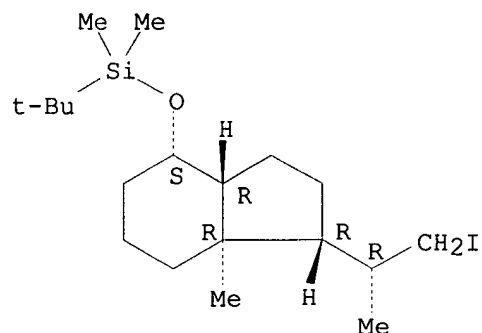
Absolute stereochemistry.



RN 214351-86-7 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[[[(1R,3aR,4S,7aR)-octahydro-1-[(1R)-2-iodo-1-methylethyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

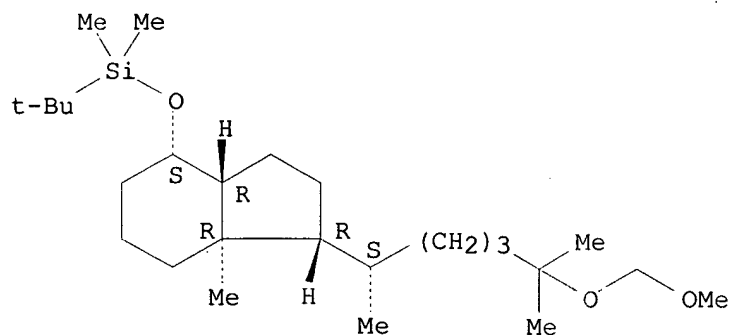
Absolute stereochemistry.



RN 214351-88-9 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[[(1R, 3aR, 4S, 7aR)-octahydro-1-[(1S)-5-(methoxymethoxy)-1,5-dimethylhexyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

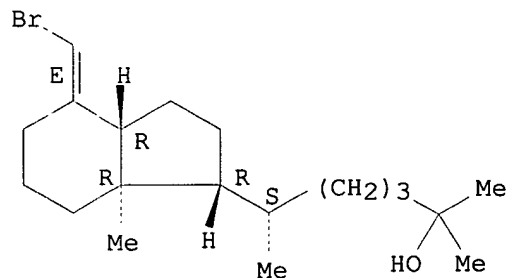


RN 214351-89-0 HCAPLUS

CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

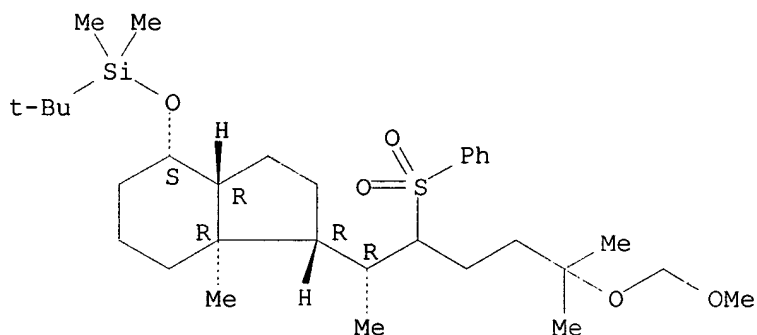


RN 214351-91-4 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[[(1R, 3aR, 4S, 7aR)-octahydro-1-[(1R)-5-

(methoxymethoxy)-1,5-dimethyl-2-(phenylsulfonyl)hexyl]-7a-methyl-1H-inden-4-yl]oxy]- (9CI) (CA INDEX NAME)

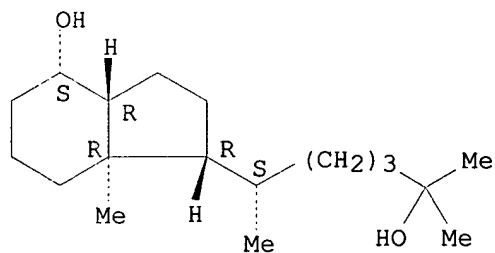
Absolute stereochemistry.



RN 214351-92-5 HCAPLUS

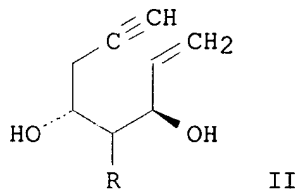
CN 1H-Indene-1-pentanol, octahydro-4-hydroxy-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.S,1R,3aR,4S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



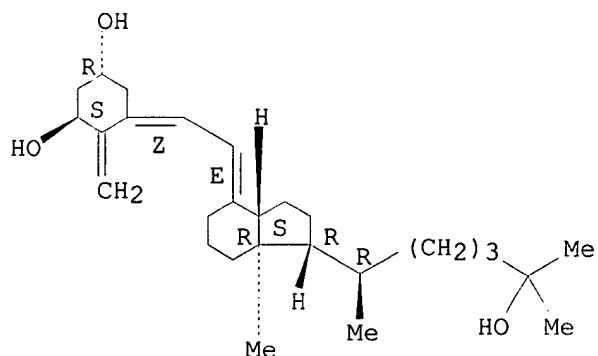
=> D L6 BIB ABS HITSTR 3

L6 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 1999 ACS
AN 1998:85846 HCAPLUS
DN 128:180577
TI A novel and practical route to A-ring enyne synthon for
1.alpha.,25-dihydroxyvitamin D3 analogs: synthesis of A-ring
diastereomers
of 1.alpha.,25-dihydroxyvitamin D3 and 2-methyl-1,25-dihydroxyvitamin D3
AU Konno, Katsuhiko; Maki, Shojiro; Fujishima, Toshie;
Liu, Zhaopeng; Miura, Daishiro; Chokki, Manabu; Takayama, Hiroaki
CS Faculty Pharmaceutical Sciences, Teikyo Univ., Sagamiko, Kanagawa,
199-01,
Japan
SO Bioorg. Med. Chem. Lett. (1998), 8(2), 151-156
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 128:180577
GI



AB A novel and practical route to the A-ring enyne synthon II (R = H, Me),
which can be versatile for a variety of A-ring analogs of
1.alpha.,25-dihydroxyvitamin D3 (I), was developed. This novel method
led
to an improved synthesis of the A-ring diastereomers of I, and synthesis
of the new analogs, 2-methyl-1,25-dihydroxyvitamin D3 with its all
possible diastereomers. The biol. evaluation of the 2-Me analogs showed
the .alpha..alpha..beta.-isomer to be more potent than I.
IT 32222-06-3DP, 1.alpha.,25-Dihydroxyvitamin D3, A-ring analogs
158388-11-5P 203126-73-2P 203126-91-4P
203126-92-5P 203126-93-6P 203126-94-7P
203126-95-8P 203126-96-9P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3
analog)
RN 32222-06-3 HCAPLUS
CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol,
(1.alpha.,3.beta.,5Z,7E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

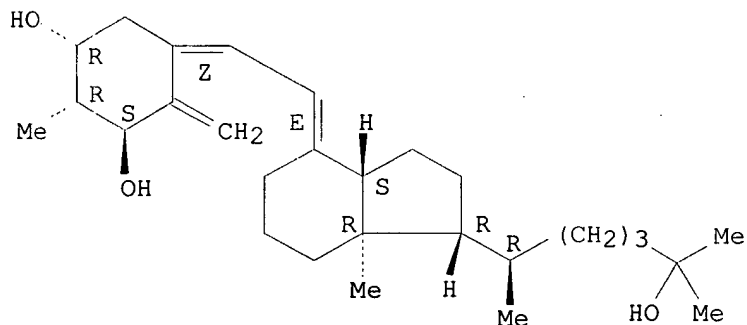


RN 158388-11-5 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

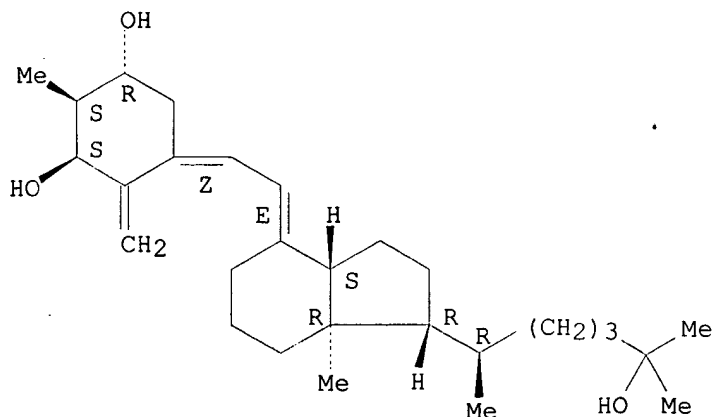


RN 203126-73-2 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

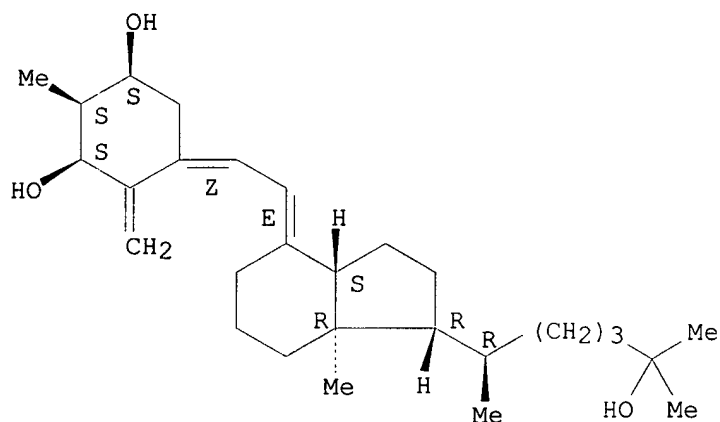


RN 203126-91-4 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

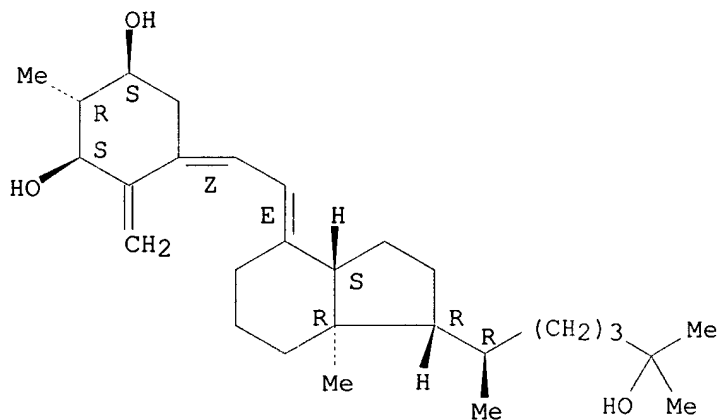


RN 203126-92-5 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.alpha.,2.beta.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

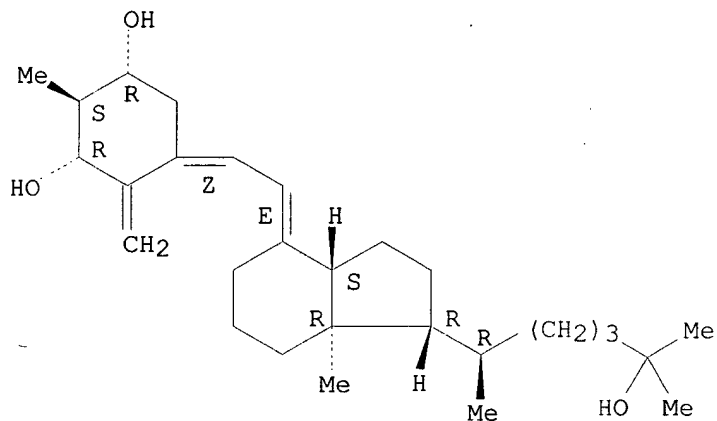


RN 203126-93-6 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.beta.,2.alpha.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

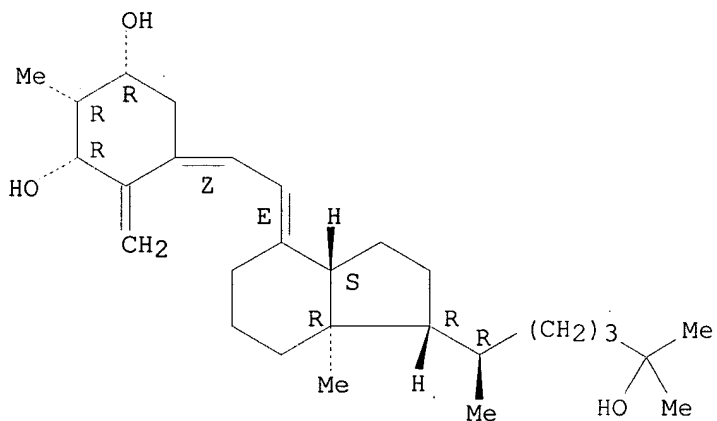


RN 203126-94-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.β.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

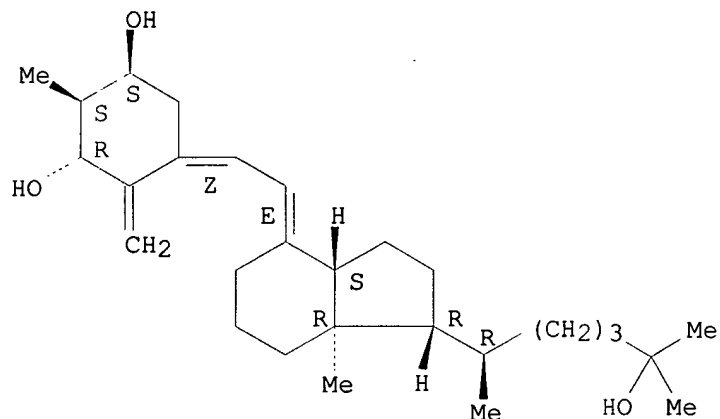


RN 203126-95-8 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.α.,3.α.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

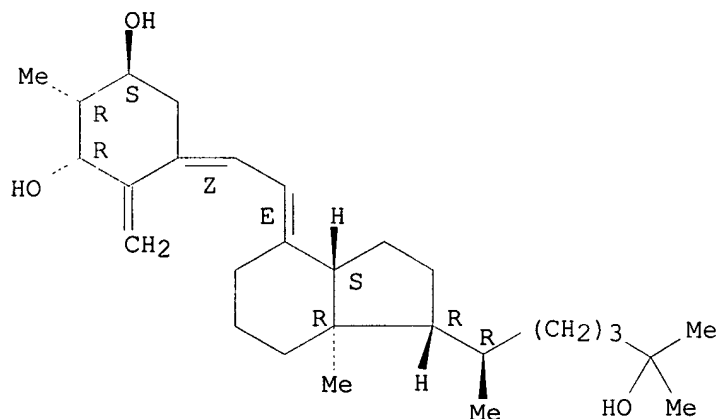


RN 203126-96-9 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 2-methyl-,
(1.β.,2.β.,3.α.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



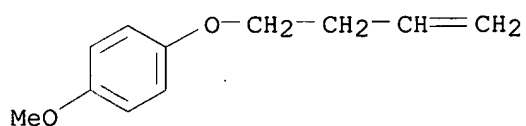
IT 2653-90-9 72657-23-9, Methyl (R)-3-hydroxy-2-methylpropionate 80657-57-4, Methyl (S)-3-hydroxy-2-methylpropionate 143705-63-9

RL: RCT (Reactant)

(prepn. of A-ring enyne synthons and 1.α.,25-dihydroxyvitamin D3 analogs)

RN 2653-90-9 HCAPLUS

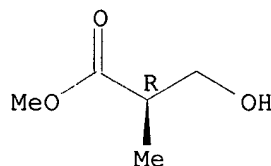
CN Benzene, 1-(3-butenyloxy)-4-methoxy- (7CI, 9CI) (CA INDEX NAME)



RN 72657-23-9 HCAPLUS

CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

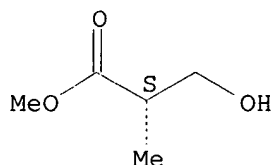
Absolute stereochemistry. Rotation (-).



RN 80657-57-4 HCAPLUS

CN Propanoic acid, 3-hydroxy-2-methyl-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

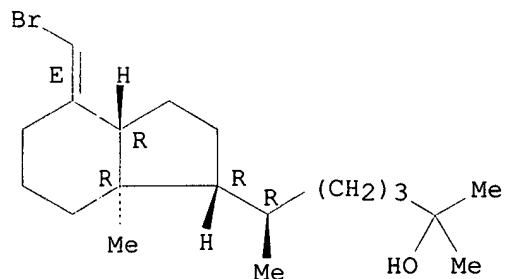
Absolute stereochemistry. Rotation (+).



RN 143705-63-9 HCAPLUS

CN 1H-Indene-1-pentanol, 4-(bromomethylene)octahydro-.alpha.,.alpha.,.epsilon.,7a-tetramethyl-, (.epsilon.R,1R,3aR,4E,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

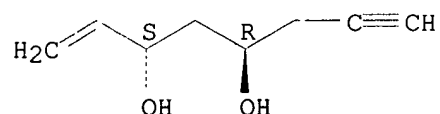


IT 152032-72-9P 161055-41-0P 169310-79-6P
169315-01-9P 203126-72-1P 203126-74-3P
203126-76-5P 203126-78-7P 203126-79-8P
203126-80-1P 203126-81-2P 203126-83-4P
203126-84-5P 203126-85-6P 203126-86-7P
203126-87-8P 203126-88-9P 203126-89-0P
203126-90-3P 203126-97-0P 203126-98-1P
203126-99-2P 203127-00-8P 203127-01-9P
203127-02-0P 203127-03-1P 203127-04-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3
analogs)

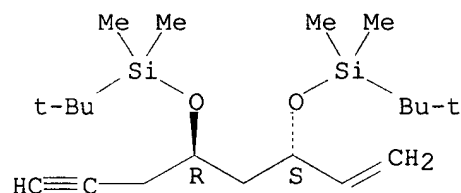
RN 152032-72-9 HCAPLUS
 CN 1-Octen-7-yne-3,5-diol, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



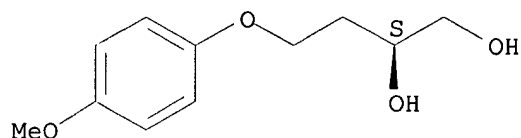
RN 161055-41-0 HCAPLUS
 CN 4,8-Dioxa-3,9-disilaundecane,
 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-
 propynyl)-, (5S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



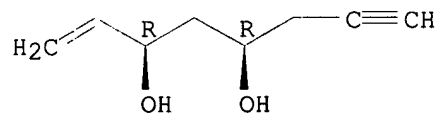
RN 169310-79-6 HCAPLUS
 CN 1,2-Butanediol, 4-(4-methoxyphenoxy)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



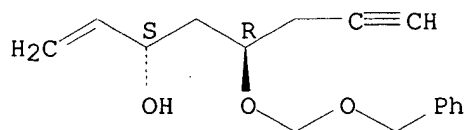
RN 169315-01-9 HCAPLUS
 CN 1-Octen-7-yne-3,5-diol, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 203126-72-1 HCAPLUS
 CN 1-Octen-7-yn-3-ol, 5-[(phenylmethoxy)methoxy]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

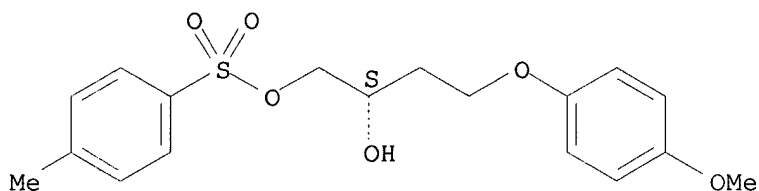
Absolute stereochemistry. Rotation (-).



RN 203126-74-3 HCAPLUS

CN 1,2-Butanediol, 4-(4-methoxyphenoxy)-, 1-(4-methylbenzenesulfonate), (S)- (9CI) (CA INDEX NAME)

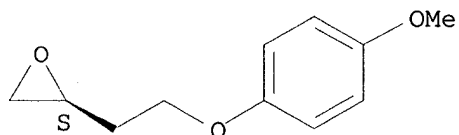
Absolute stereochemistry. Rotation (+).



RN 203126-76-5 HCAPLUS

CN Oxirane, [2-(4-methoxyphenoxy)ethyl]-, (S)- (9CI) (CA INDEX NAME)

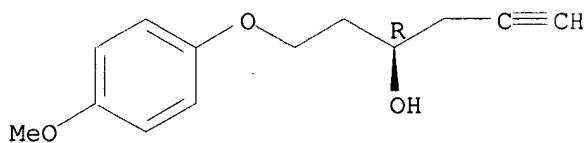
Absolute stereochemistry. Rotation (-).



RN 203126-78-7 HCAPLUS

CN 5-Hexyn-3-ol, 1-(4-methoxyphenoxy)-, (R)- (9CI) (CA INDEX NAME)

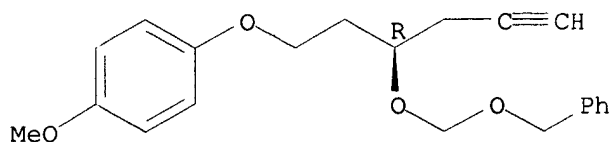
Absolute stereochemistry. Rotation (-).



RN 203126-79-8 HCAPLUS

CN Benzene, 1-methoxy-4-[[3-[(phenylmethoxy)methoxy]-5-hexynyl]oxy]-, (R)- (9CI) (CA INDEX NAME)

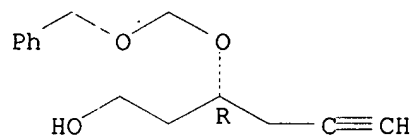
Absolute stereochemistry. Rotation (-).



RN 203126-80-1 HCAPLUS

CN 5-Hexyn-1-ol, 3-[(phenylmethoxy)methoxy]-, (R)- (9CI) (CA INDEX NAME)

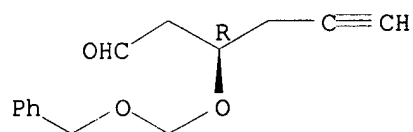
Absolute stereochemistry. Rotation (-).



RN 203126-81-2 HCAPLUS

CN 5-Hexynal, 3-[(phenylmethoxy)methoxy]-, (R)- (9CI) (CA INDEX NAME)

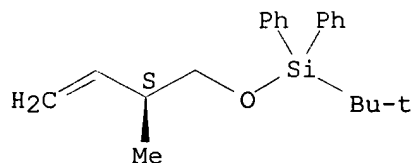
Absolute stereochemistry.



RN 203126-83-4 HCAPLUS

CN Silane, (1,1-dimethylethyl)[(2-methyl-3-butenyl)oxy]diphenyl-, (S)- (9CI)
(CA INDEX NAME)

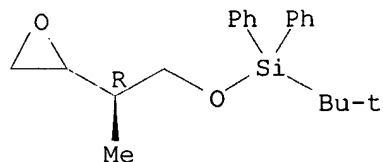
Absolute stereochemistry. Rotation (-).



RN 203126-84-5 HCAPLUS

CN Silane, (1,1-dimethylethyl)(2-oxiranylpropoxy)diphenyl-, [2(R)]- (9CI)
(CA INDEX NAME)

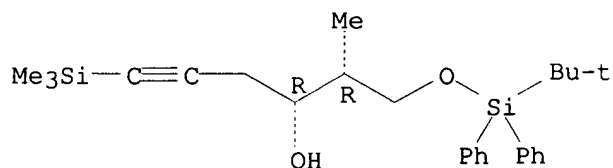
Absolute stereochemistry.



RN 203126-85-6 HCAPLUS

CN 5-Hexyn-3-ol, 1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-(trimethylsilyl)-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

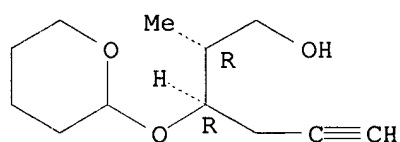
Absolute stereochemistry. Rotation (+).



RN 203126-86-7 HCAPLUS

CN 5-Hexyn-1-ol, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-,
[2(2R,3R)]-[partial]- (9CI) (CA INDEX NAME)

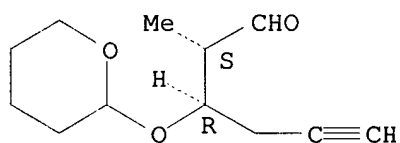
Absolute stereochemistry.



RN 203126-87-8 HCAPLUS

CN 5-Hexynal, 2-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]-,
[2(2S,3R)]-[partial]- (9CI) (CA INDEX NAME)

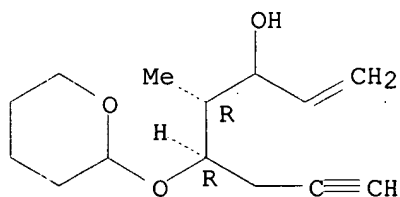
Absolute stereochemistry.



RN 203126-88-9 HCAPLUS

CN 1-Octen-7-yn-3-ol, 4-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-,
[2(4R,5R)]-[partial]- (9CI) (CA INDEX NAME)

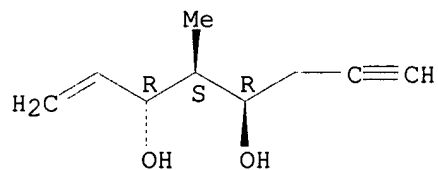
Absolute stereochemistry.



RN 203126-89-0 HCAPLUS

CN 1-Octen-7-yn-3,5-diol, 4-methyl-, [3R-(3R*,4S*,5R*)]- (9CI) (CA INDEX NAME)

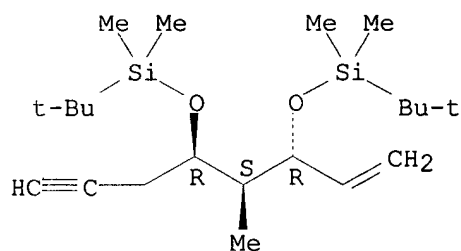
Absolute stereochemistry.



RN 203126-90-3 HCAPLUS

CN 4,8-Dioxa-3,9-disilaundecane, 5-ethenyl-2,2,3,3,6,9,9,10,10-nonamethyl-7-(2-propynyl)-, (5R,6S,7R)- (9CI) (CA INDEX NAME)

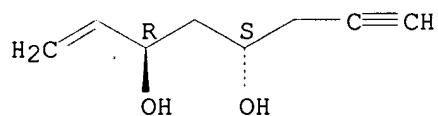
Absolute stereochemistry. Rotation (+).



RN 203126-97-0 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

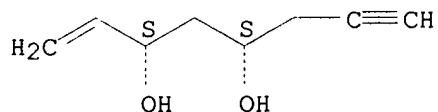
Absolute stereochemistry.



RN 203126-98-1 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

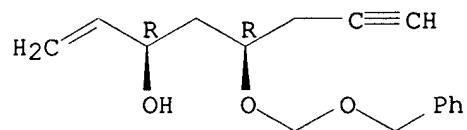
Absolute stereochemistry.



RN 203126-99-2 HCAPLUS

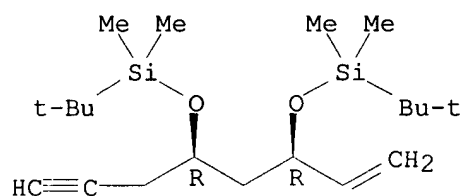
CN 1-Octen-7-yn-3-ol, 5-[(phenylmethoxy)methoxy]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



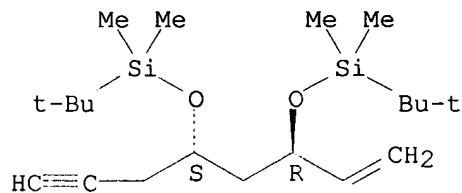
RN 203127-00-8 HCAPLUS
 CN 4,8-Dioxa-3,9-disilaundecane,
 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-
 propynyl)-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



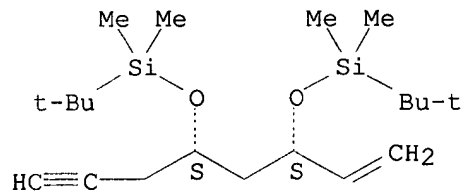
RN 203127-01-9 HCAPLUS
 CN 4,8-Dioxa-3,9-disilaundecane,
 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-
 propynyl)-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



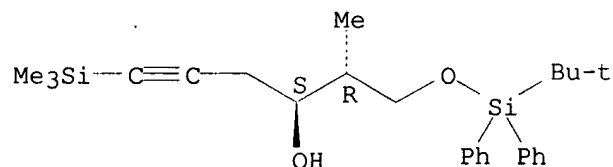
RN 203127-02-0 HCAPLUS
 CN 4,8-Dioxa-3,9-disilaundecane,
 5-ethenyl-2,2,3,3,9,9,10,10-octamethyl-7-(2-
 propynyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 203127-03-1 HCAPLUS
 CN 5-Hexyn-3-ol, 1-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methyl-6-
 (trimethylsilyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

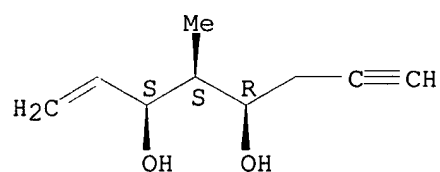
Absolute stereochemistry. Rotation (-).



RN 203127-04-2 HCAPLUS

CN 1-Octen-7-yne-3,5-diol, 4-methyl-, [3S-(3R*,4R*,5S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 61476-45-7P 66791-71-7P 96614-28-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

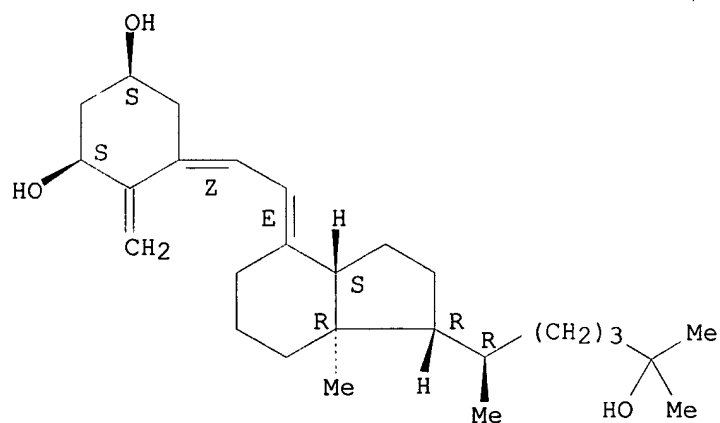
(prepn. of A-ring enyne synthons and 1.alpha.,25-dihydroxyvitamin D3 analogs)

RN 61476-45-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.alpha.,3.alpha.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

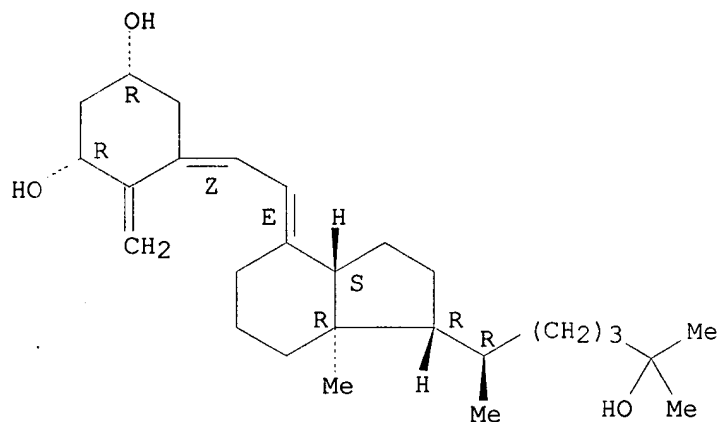


RN 66791-71-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, (1.beta.,3.beta.,5Z,7E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



RN 96614-28-7 HCAPLUS

CN 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol,
(1.β.,3.α.,5Z,7E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

